Electronic supplementary information

Cascade reaction of β,γ-unsaturated α-ketoesters with phenols in trityl chloride/TFA system. Highly selective synthesis of 4-aryl-2*H*-chromenes and their applications

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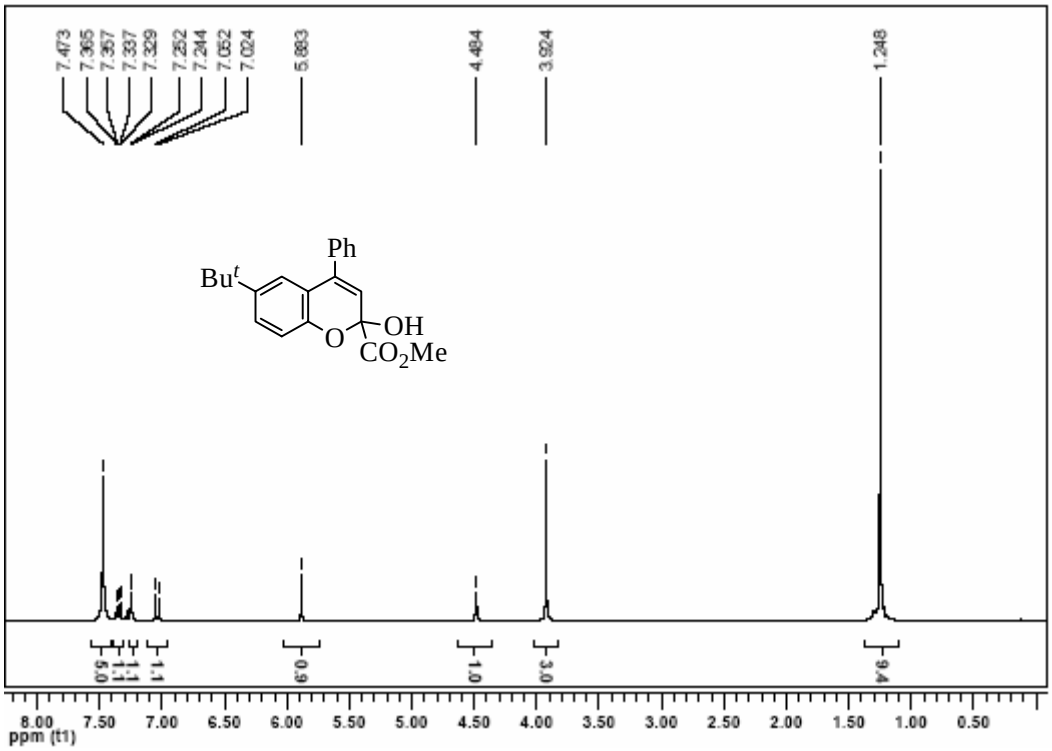
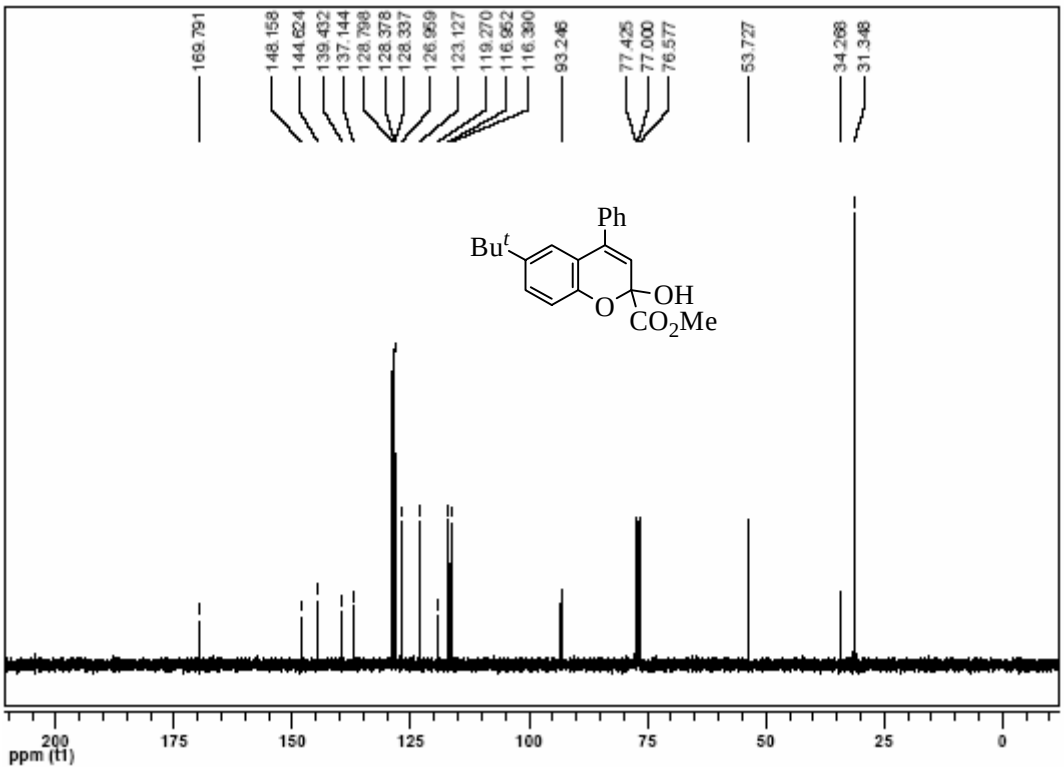
1.1. ^{1}H and ^{13}C NMR spectra of 4-aryl-2*H*-chromenes **3**

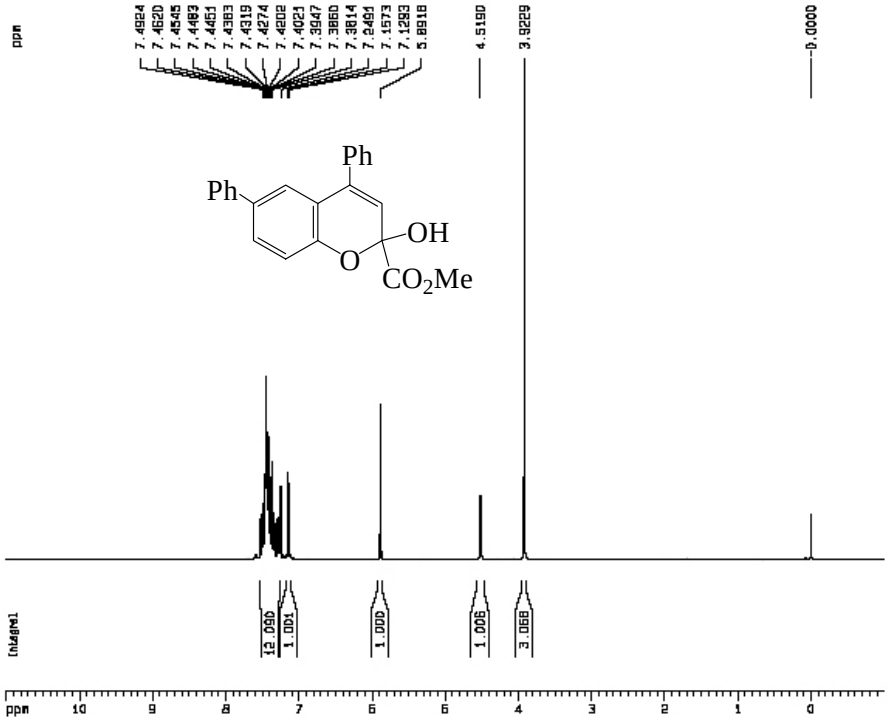
4-Aryl-2*H*-chromene **3a**: ^{1}H NMR (300MHz, $CDCl_3$)



4-Aryl-2*H*-chromene **3a**: ^{13}C NMR (75MHz, $CDCl_3$)



4-Aryl-2*H*-chromene **3b**: ^{1}H NMR (300MHz, $CDCl_3$)



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D1 1.00000000 sec

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F2P -1.000 ppm
F2 -300.13 Hz
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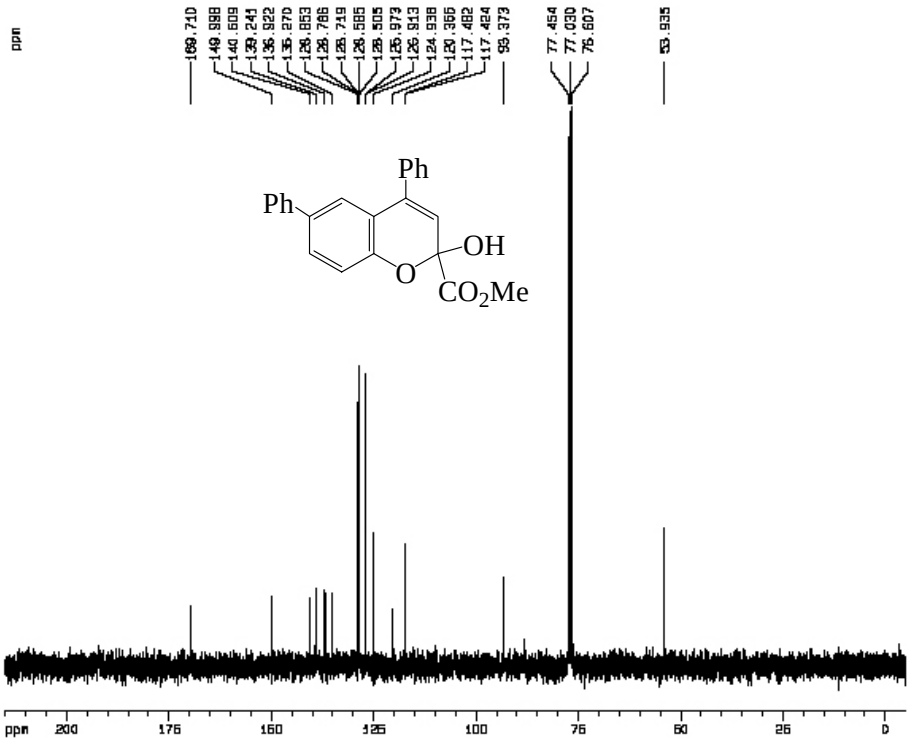
HZCM 180.07800 Hz/cm

4-Aryl-2*H*-chromene **3b**: ^{13}C NMR (75MHz, $CDCl_3$)



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SOLVENT CDCl3
NS 80
DS 4
SWH 17980.514 Hz
FIDRES 0.274456 Hz
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RG 456.1
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d12 0.00002000 sec

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CHANNEL f2
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1D NMR plot parameters
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F1 18325.57 Hz
F2P -5.000 ppm
F2 -377.34 Hz
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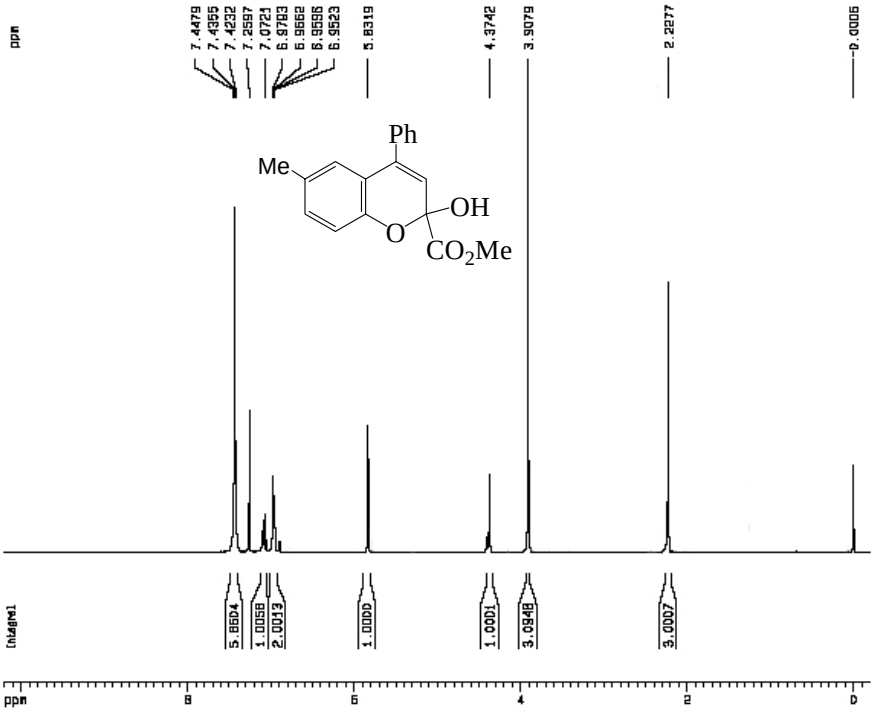
4-Aryl-2*H*-chromene **3c**: ^{1}H NMR (300MHz, $CDCl_3$)



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PROCNO 1

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TE 281.5 K
D1 2.00000000 sec

CHANNEL f1
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P1 9.30 usec
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LB 0.30 Hz
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1D NMR plot parameters
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CY 12.60 cm
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F2P -0.200 ppm
F2 -60.03 Hz
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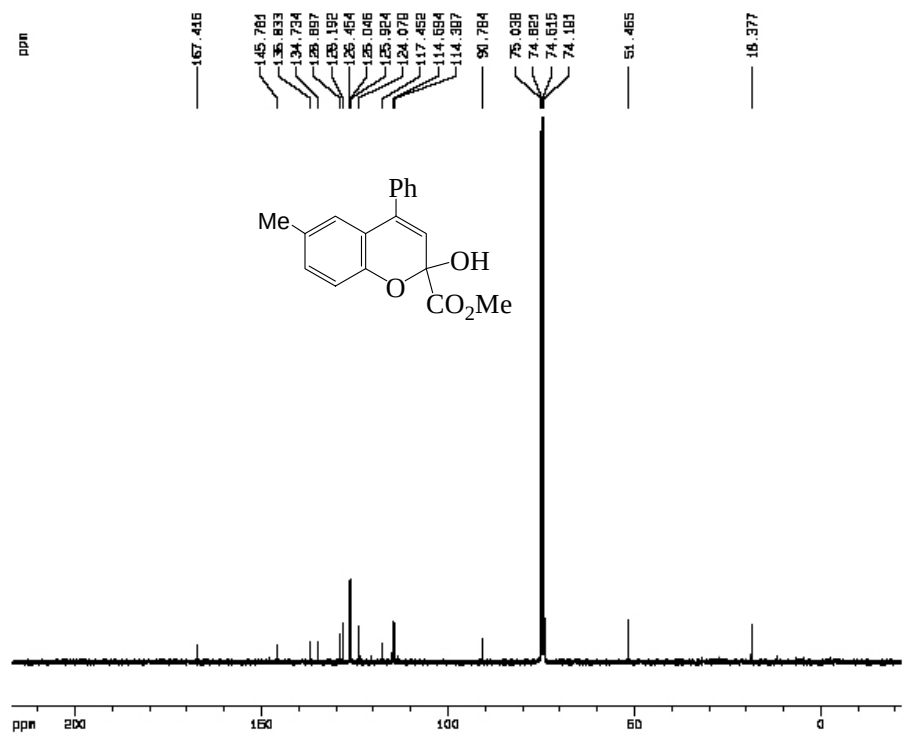
4-Aryl-2*H*-chromene **3c**: ^{13}C NMR (75MHz, $CDCl_3$)



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FIDRES 0.274458 Hz
AQ 1.8218508 sec
RG 1825.6
DW 27.800 usec
DE 6.00 usec
TE 291.7 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00020000 sec

CHANNEL f1
NUC1 13C
P1 9.40 usec
PL1 -1.00 dB
SFO1 75.4752953 MHz

CHANNEL f2
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NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 15.00 dB
PL13 15.00 dB
SFO2 300.1312005 MHz

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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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F1 18355.80 Hz
F2P -21.596 ppm
F2 -1639.78 Hz
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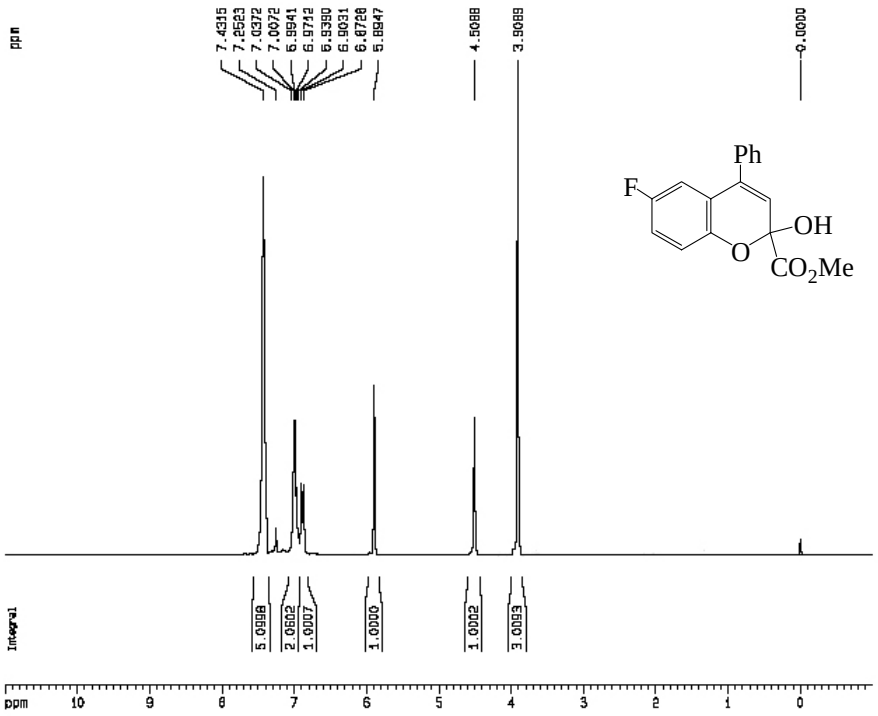


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TD                 65536
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DS                     2
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FIDRES          0.094190 Hz
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RG                   181
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TE                295.6 K
D1             2.00000000 sec

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PL1                0.00 dB
SFO1        300.1318634 MHz

F2 - Processing parameters
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SF          300.1300000 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00

1D NMR plot parameters
CX                20.00 cm
CY                12.50 cm
F1P              11.000 ppm
F1                3301.43 Hz
F2P              -1.000 ppm
F2                -300.13 Hz
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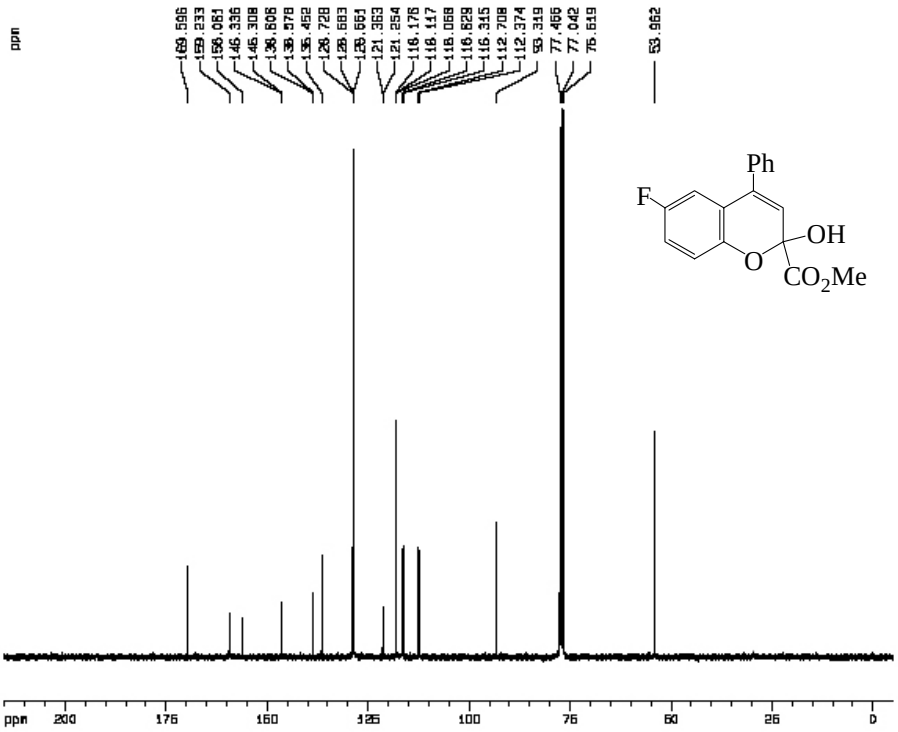
4-Aryl-2*H*-chromene **3d**: ^{13}C NMR (75MHz, $CDCl_3$)

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EXPNO                 11
PROCNO                 1

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PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  2000
DS                     4
SWH             17985.614 Hz
FIDRES          0.274438 Hz
AQ              1.8249508 sec
RG                  3251
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TE                297.0 K
D1             2.00000000 sec
d11            0.03000000 sec
d12            0.00002000 sec

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======== CHANNEL f2 ========
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NUC2                1H
PCPD2             80.00 usec
PL2               0.00 dB
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PL13              17.70 dB
SFO2        300.1312000 MHz

F2 - Processing parameters
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SF          75.4577490 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40

1D NMR plot parameters
CX                20.00 cm
CY                12.50 cm
F1P             215.000 ppm
F1              16225.57 Hz
F2P              -5.000 ppm
F2               -377.34 Hz
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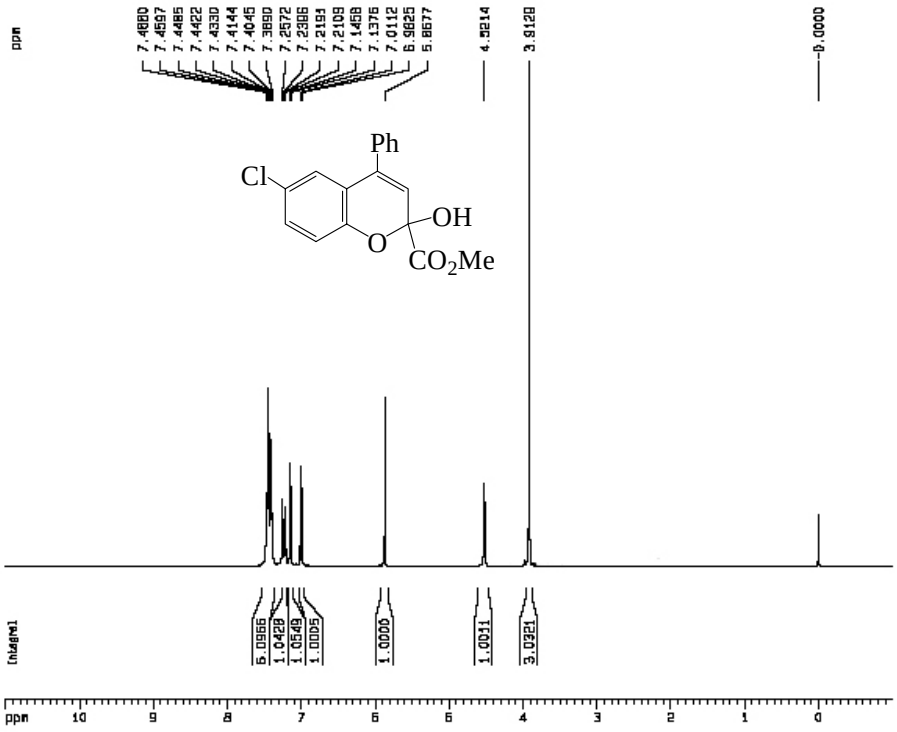
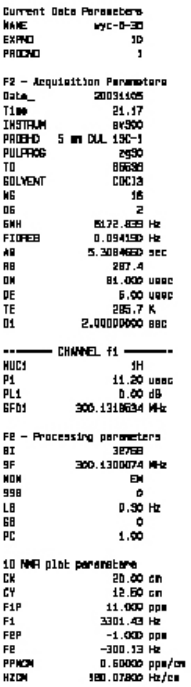
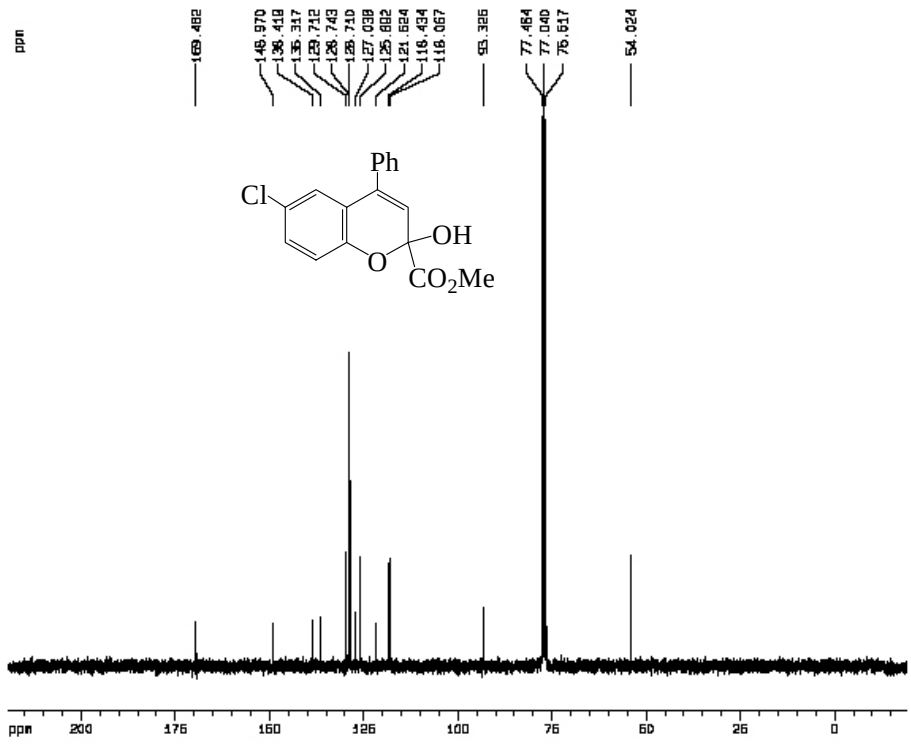
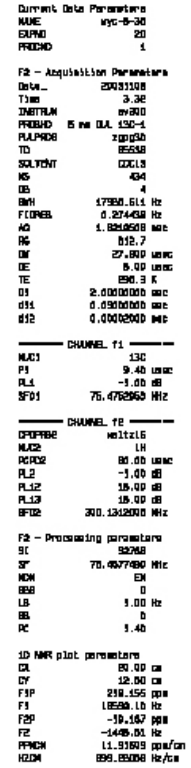
4-Aryl-2*H*-chromene **3e**: ^{1}H NMR (300MHz, $CDCl_3$)



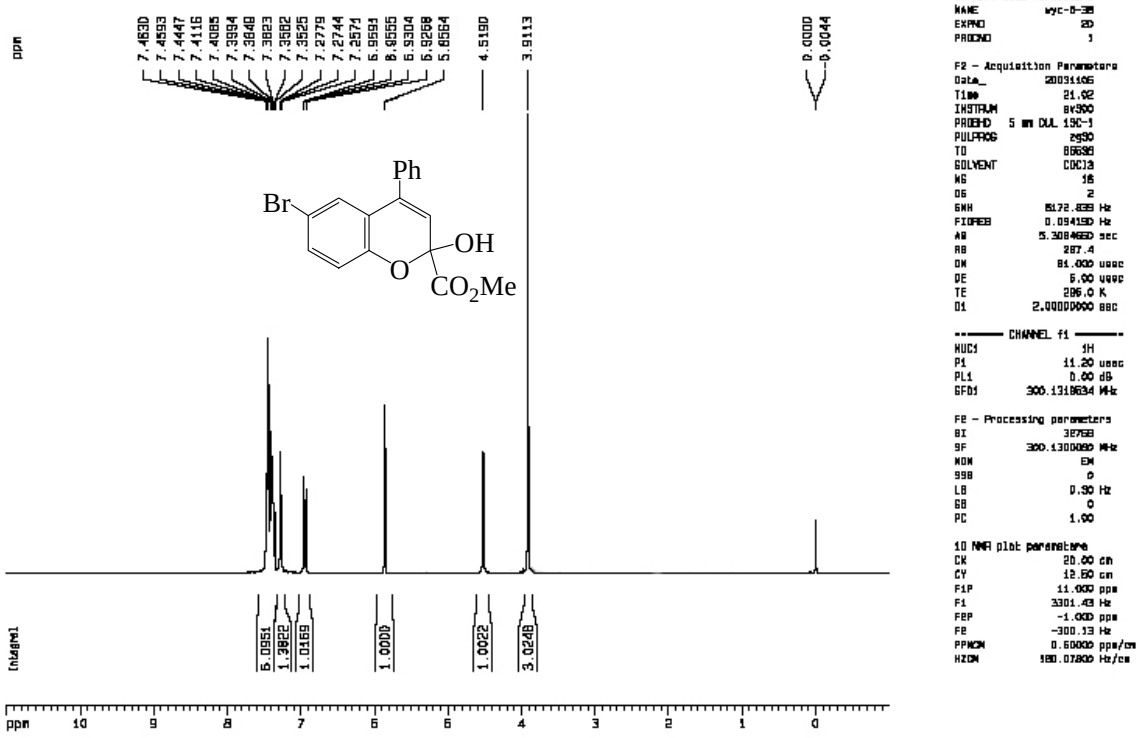


4-Aryl-2*H*-chromene **3e**: ^{13}C NMR (75MHz, $CDCl_3$)

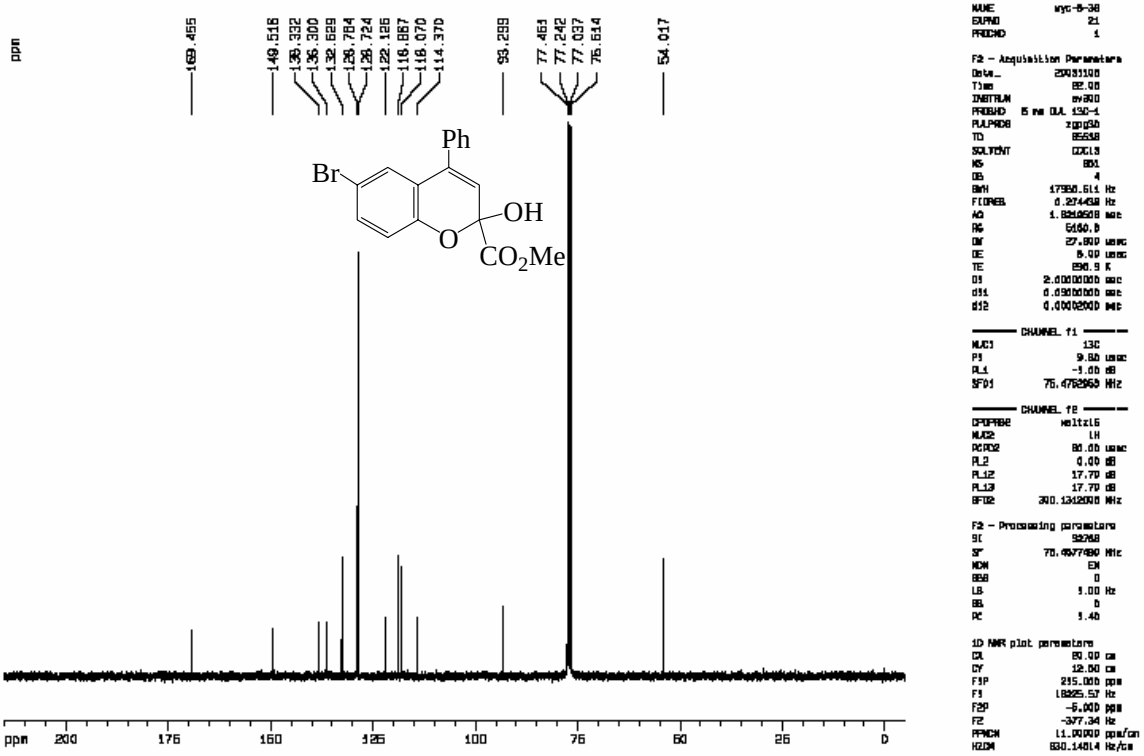




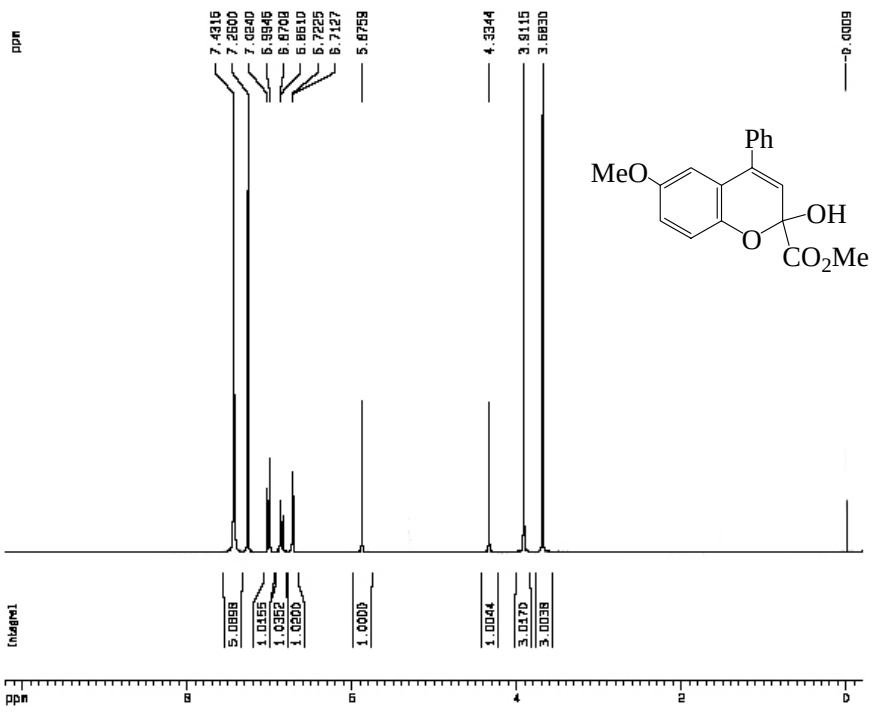
4-Aryl-2*H*-chromene **3f**: ^{1}H NMR (300MHz, $CDCl_3$)



4-Aryl-2*H*-chromene **3f**: ^{13}C NMR (75MHz, $CDCl_3$)



4-Aryl-2*H*-chromene **3g**: ^{1}H NMR (300MHz, $CDCl_3$)

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RG                    512
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TE                 285.9 K
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F2                 -60.03 Hz
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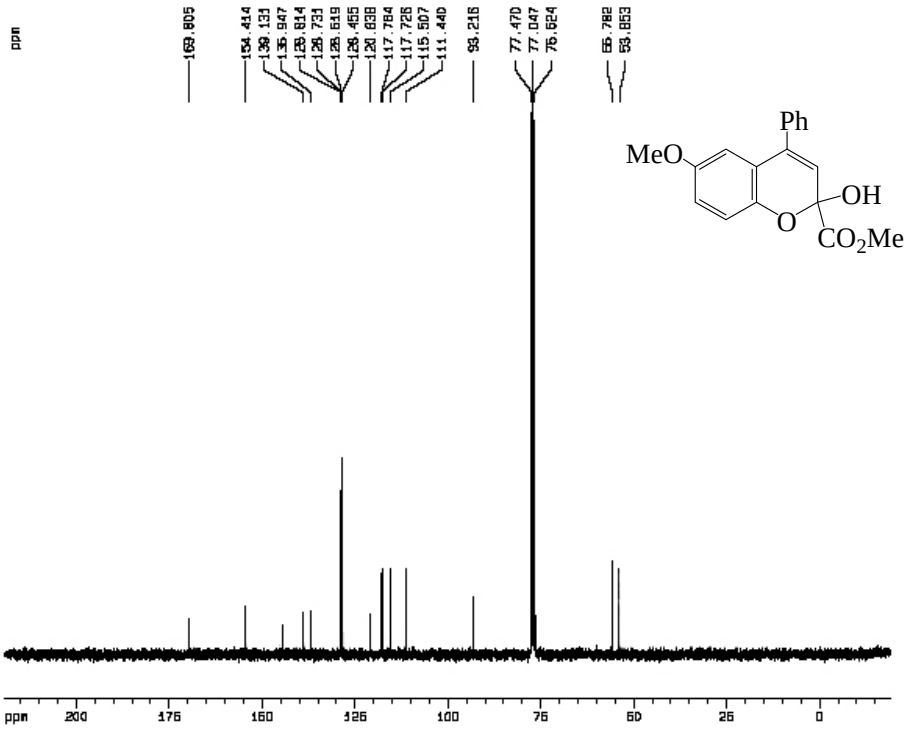
4-Aryl-2*H*-chromene **3g**: ^{13}C NMR (75MHz, $CDCl_3$)

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PROCNO                      1

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TD                 65536
SOLVENT             CDCl3
NS                    387
DS                      4
SWH              17960.611 Hz
FIDRES           0.274150 Hz
AQ               1.8218598 sec
RG                 1625.5
DW                 27.800 usec
DE                 6.00 usec
TE                 295.3 K
D1              2.00000000 sec
D11             0.03000000 sec
D12             0.00002000 sec

======== CHANNEL f1 ========
NUC1                   13C
P1                  9.60 usec
PL1                 -1.00 dB
SFO1          75.4752693 MHz

======== CHANNEL f2 ========
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NUC2                   1H
PCPD2               80.00 usec
PL2                 0.00 dB
PL12                17.70 dB
PL13                17.70 dB
SFO2          300.1318000 MHz

F2 - Processing parameters
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SF            75.4677400 MHz
WDW                    EM
SSB                     0
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1D NMR plot parameters
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F2P                -18.107 ppm
F2                 -1446.01 Hz
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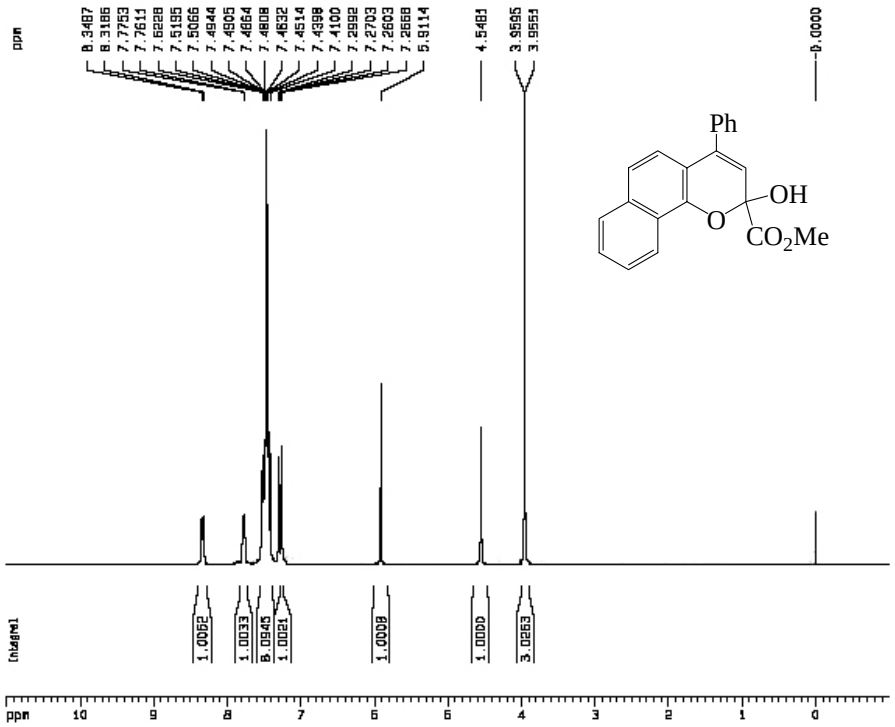
4-Aryl-2*H*-chromene **3h**: ^{1}H NMR (300MHz, $CDCl_3$)

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PULPROG          zg30
TD              86698
SOLVENT          CDCl3
NS                  16
DS                   2
SWH           6172.839 Hz
FIDRES        0.094159 Hz
AQ            5.3084650 sec
RG                 362
DW              81.000 usec
DE               6.00 usec
TE              285.9 K
D1            2.00000000 sec

======== CHANNEL f1 ========
NUC1                1H
P1               11.20 usec
PL1               0.00 dB
SFO1        300.1318634 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300059 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00

1D NMR plot parameters
CX                20.00 cm
CY                12.50 cm
F1P              11.000 ppm
F1             3301.43 Hz
F2P              -1.000 ppm
F2              -300.13 Hz
PPMCM            0.60000 ppm/cm
HZCM           180.07800 Hz/cm
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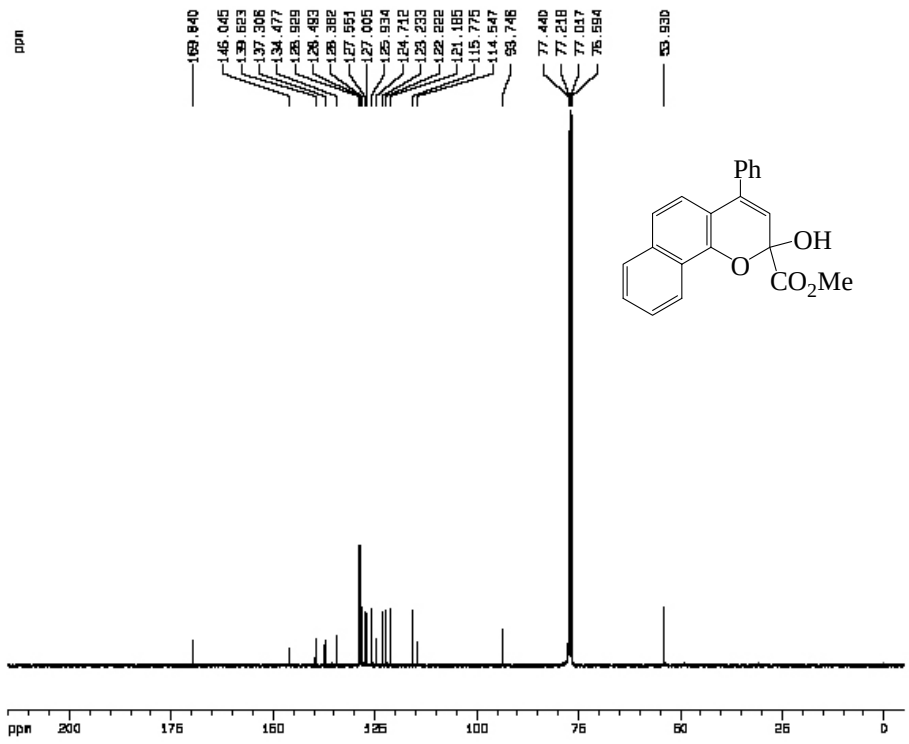
4-Aryl-2*H*-chromene **3h**: ^{13}C NMR (75MHz, $CDCl_3$)

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PROCNO                 1

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PULPROG          zgpg30
TD              65536
SOLVENT          CDCl3
NS                7142
DS                   4
SWH           17980.614 Hz
FIDRES        0.274438 Hz
AQ            1.8218508 sec
RG                3261
DW              27.800 usec
DE               6.00 usec
TE              297.3 K
D1            2.00000000 sec
d11           0.03000000 sec
d12           0.00002000 sec

======== CHANNEL f1 ========
NUC1                13C
P1               9.80 usec
PL1              -1.00 dB
SFO1        75.4752963 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2            80.00 usec
PL2               0.00 dB
PL12             17.70 dB
PL13             17.70 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF          75.4677486 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                1.40

1D NMR plot parameters
CX                20.00 cm
CY                12.50 cm
F1P             215.000 ppm
F1            16225.57 Hz
F2P              -5.000 ppm
F2             -377.34 Hz
PPMCM           11.00000 ppm/cm
HZCM          830.14032 Hz/cm
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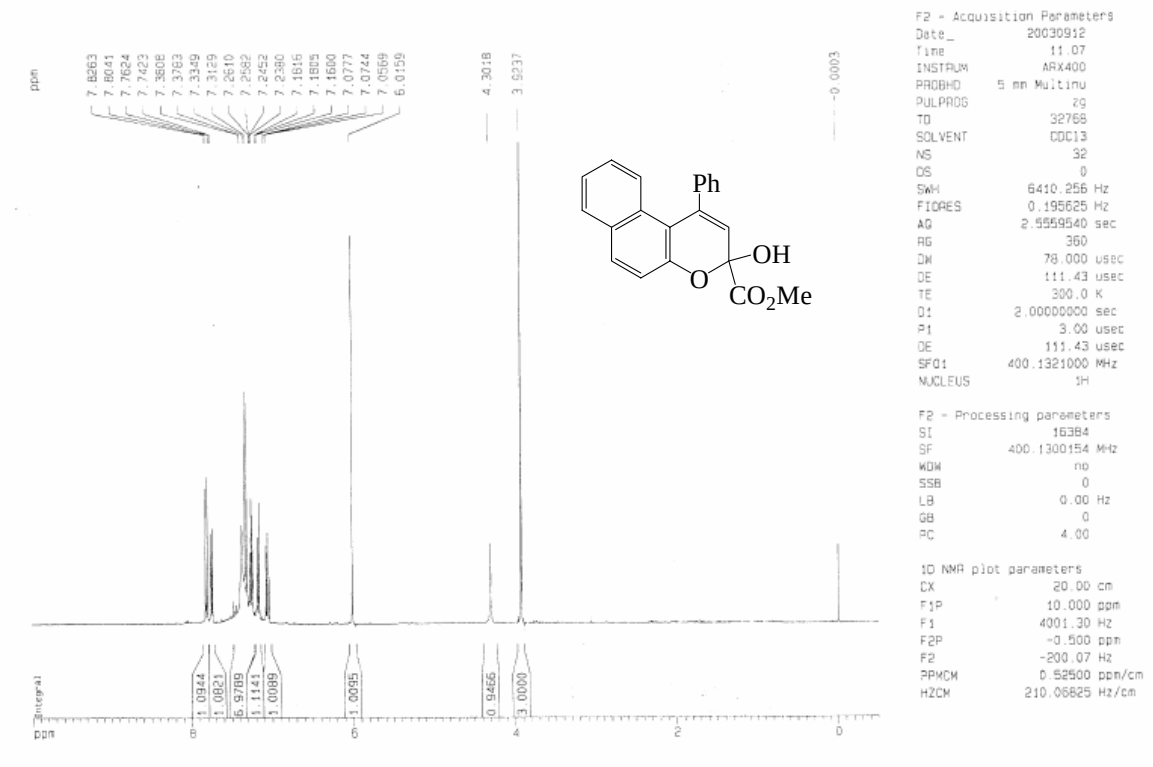
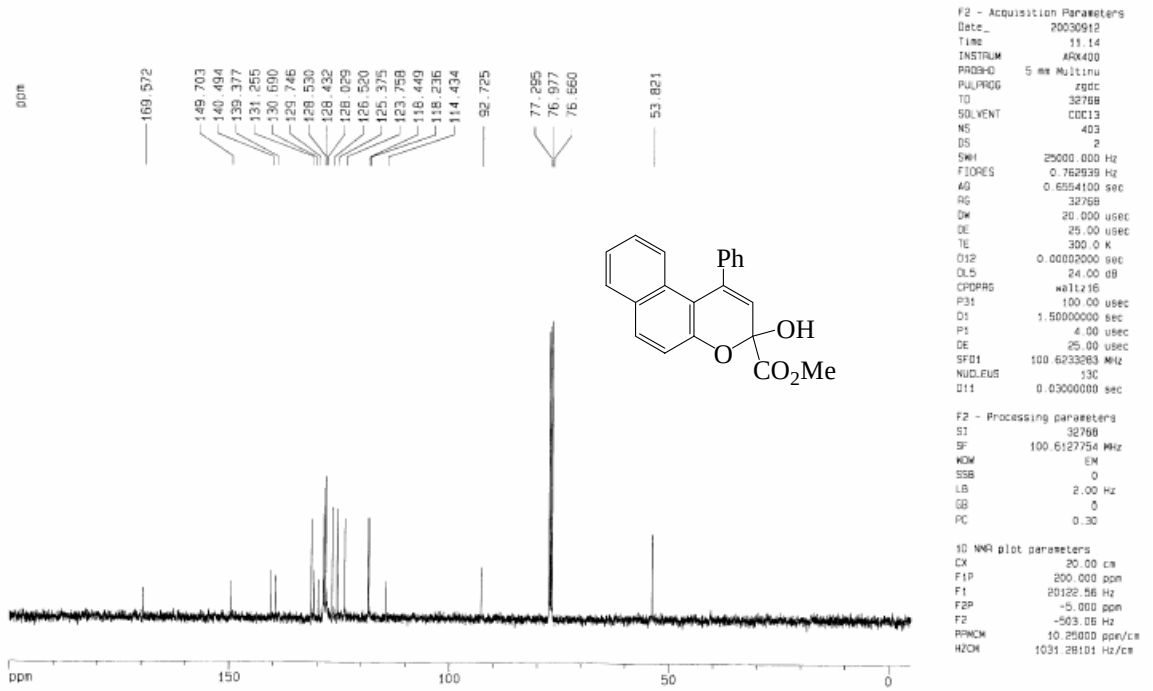
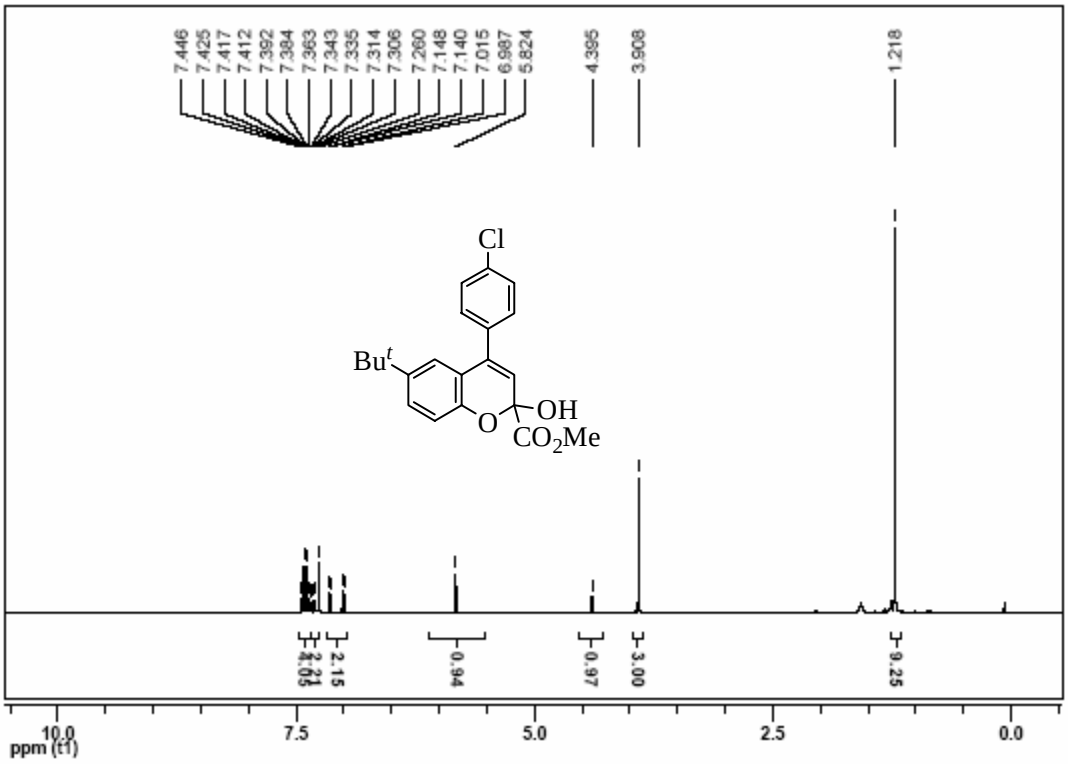
4-Aryl-2*H*-chromene **3i**: ^{1}H NMR (400MHz, $CDCl_3$)



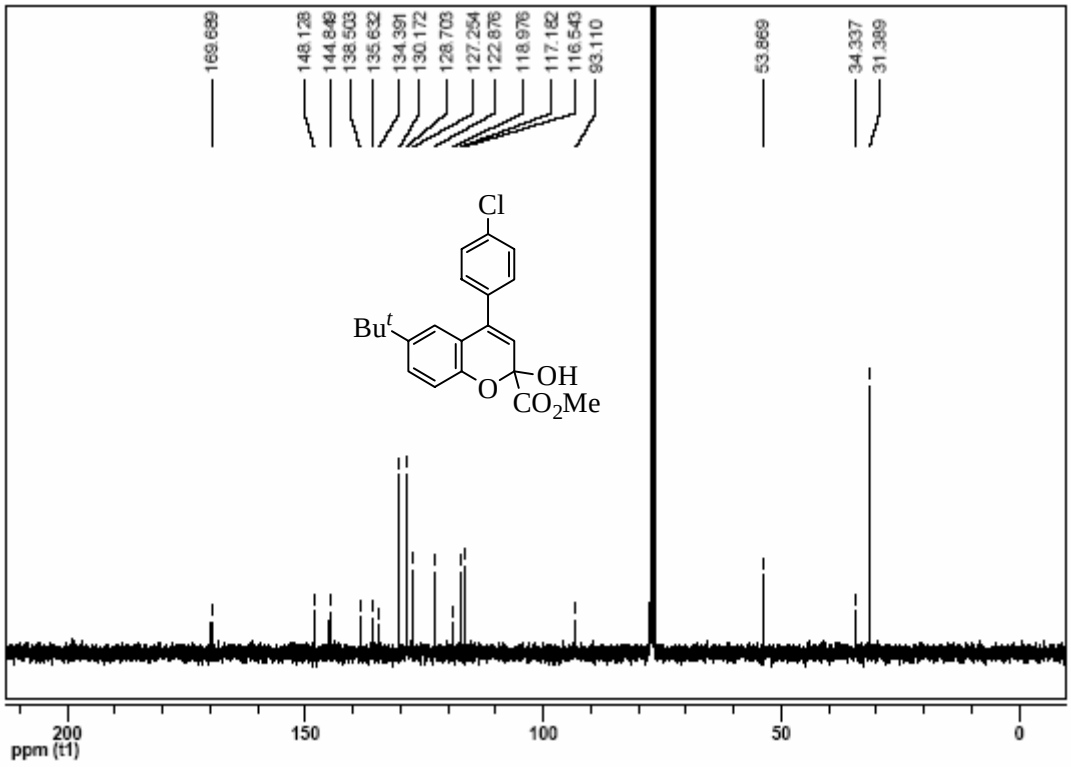
4-Aryl-2*H*-chromene **3i**: ^{13}C NMR (100MHz, $CDCl_3$)



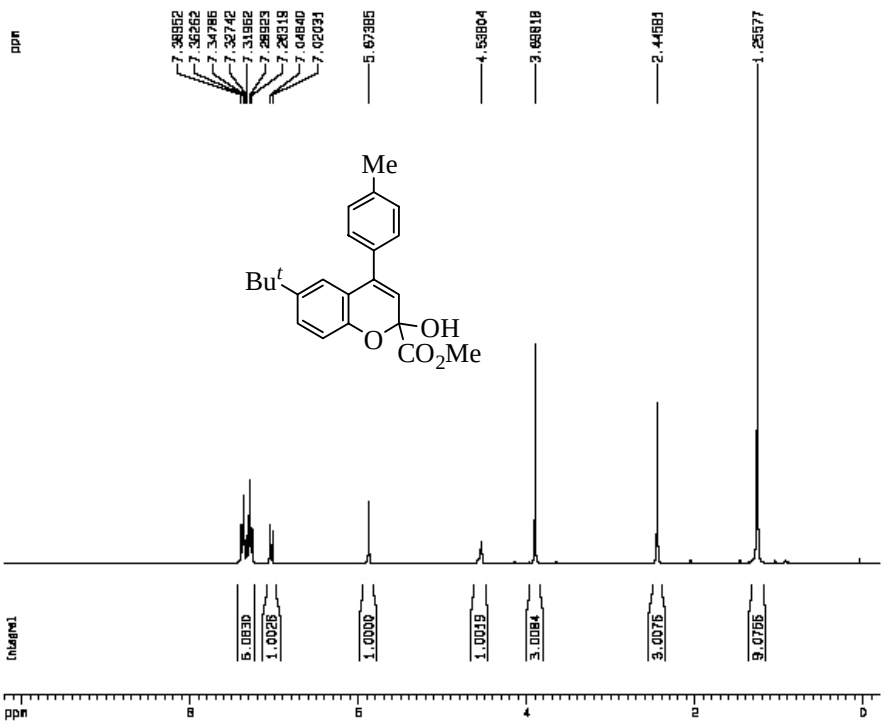
4-Aryl-2*H*-chromene **3j**: ^{1}H NMR (300MHz, $CDCl_3$)

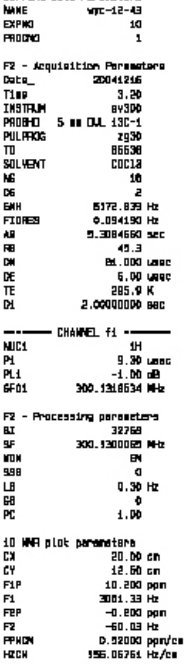


4-Aryl-2*H*-chromene **3j**: ^{13}C NMR (75MHz, $CDCl_3$)

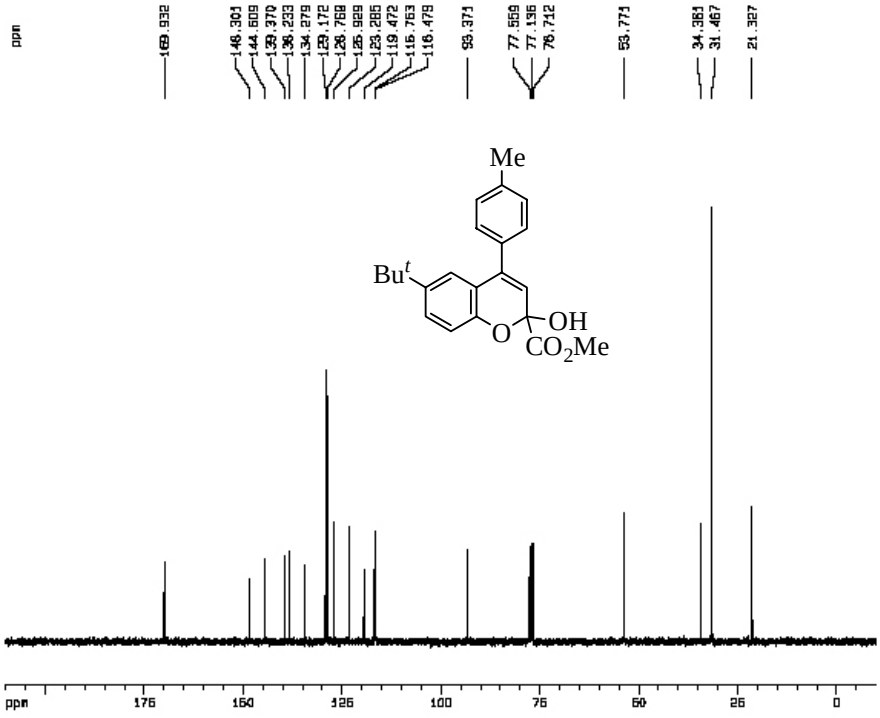


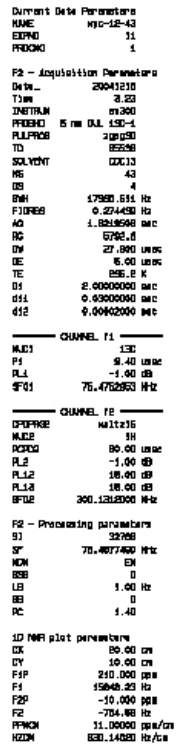
4-Aryl-2*H*-chromene **3k**: ^{1}H NMR (300MHz, $CDCl_3$)



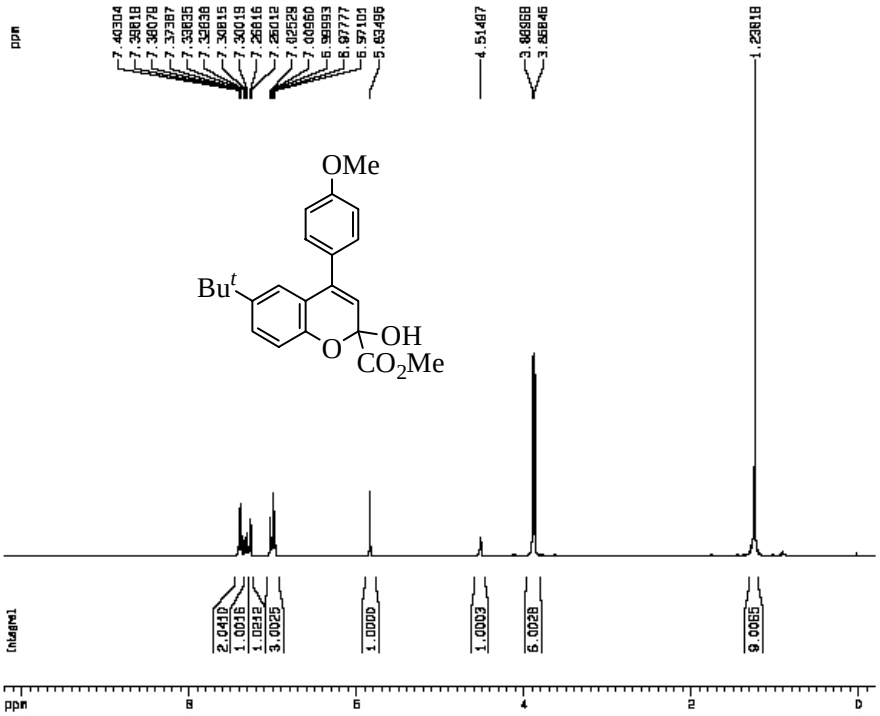


4-Aryl-2*H*-chromene **3k**: ^{13}C NMR (75MHz, $CDCl_3$)





4-Aryl-2*H*-chromene **3l**: ^{1}H NMR (300MHz, $CDCl_3$)



Current Data Parameters
NAME wyc-10-7
EXPNO 10
PROCNO 1

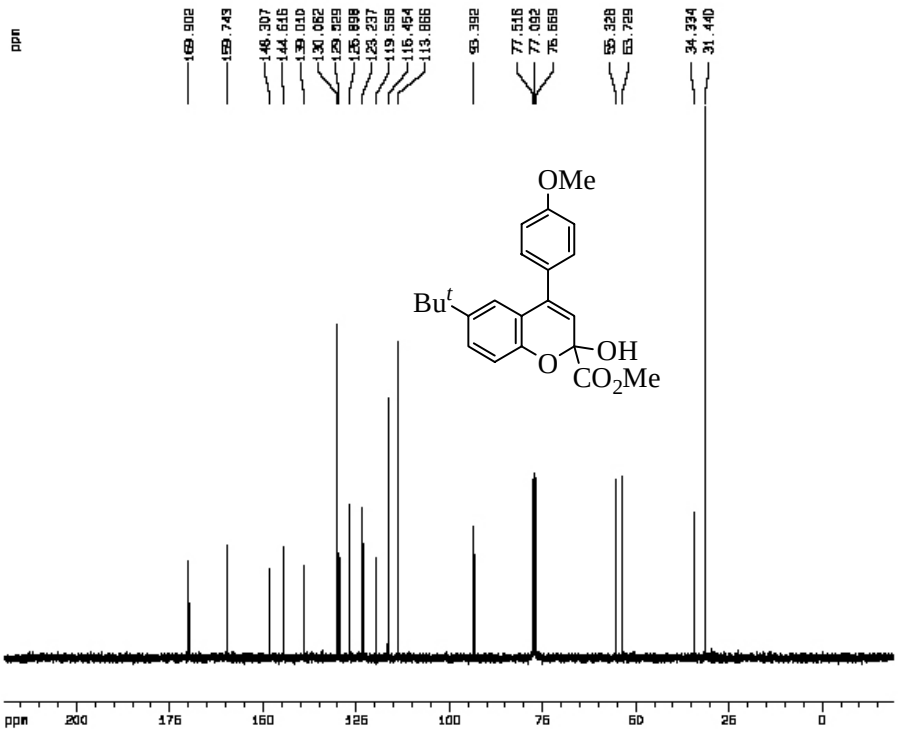
F2 - Acquisition Parameters
Date_ 20040518
Time 20.47
INSTRUM av300
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 64
DW 81.000 usec
DE 6.00 usec
TE 298.2 K
D1 2.00000000 sec

CHANNEL f1
NUC1 1H
P1 9.30 usec
PL1 -1.00 dB
SFO1 300.1318634 MHz

F2 - Processing parameters
SI 32768
SF 300.1300085 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 10.200 ppm
F1 3061.33 Hz
F2P -0.800 ppm
F2 -60.03 Hz
PPMCM 0.52000 ppm/cm
HZCM 156.06761 Hz/cm

4-Aryl-2*H*-chromene **3l**: ^{13}C NMR (75MHz, $CDCl_3$)



Current Data Parameters
NAME wyc-10-7
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040518
Time 20.51
INSTRUM av300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 68
DS 4
SWH 17985.611 Hz
FIDRES 0.274450 Hz
AQ 1.8249598 sec
RG 2580.3
DW 27.800 usec
DE 6.00 usec
TE 298.4 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

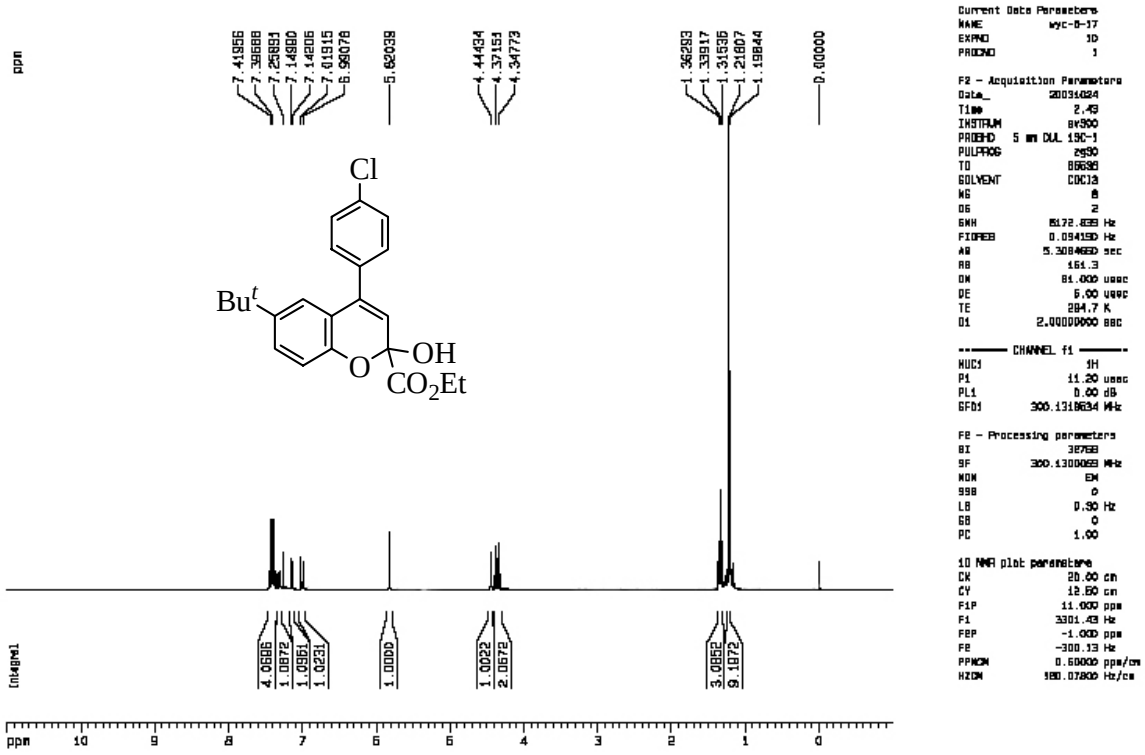
CHANNEL f1
NUC1 13C
P1 9.40 usec
PL1 -1.00 dB
SFO1 75.4752853 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 18.00 dB
PL13 18.00 dB
SFO2 300.1318000 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

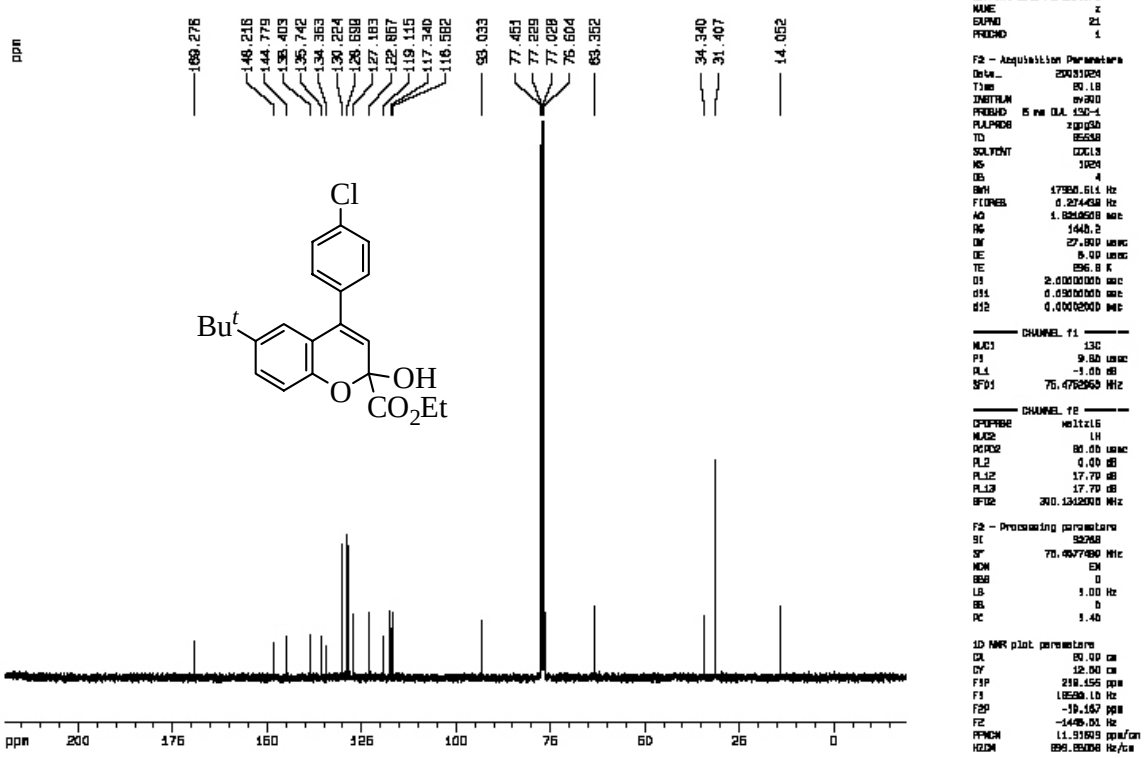
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 210.155 ppm
F1 15538.11 Hz
F2P -18.167 ppm
F2 -1445.01 Hz
PPMCM 11.91809 ppm/cm
HZCM 899.85058 Hz/cm

4-Aryl-2*H*-chromene **3m**: ^{1}H NMR (300MHz, $CDCl_3$)




```
Current Data Parameters
NAME                  wyc-8-17
EXPNO                       10
PROCNO                       1

F2 - Acquisition Parameters
Date_               20091024
Time                      2.49
INSTRUM                 av300
PROBHD   5 mm DUL 13C-1
PULPROG                 zg30
TD                      65536
SOLVENT                 CDCl3
NS                          8
DS                          2
SWH                 6172.839 Hz
FIDRES              0.094150 Hz
AQ                  5.3084650 sec
RG                      161.3
DW                     81.000 usec
DE                      6.00 usec
TE                     294.7 K
D1                  2.00000000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                      11.20 usec
PL1                      0.00 dB
SFO1            300.1318634 MHz

F2 - Processing parameters
SI                      32768
SF                300.1300069 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
PC                       1.00

1D NMR plot parameters
CX                      20.00 cm
CY                      12.60 cm
F1P                     11.000 ppm
F1                    3301.43 Hz
F2P                    -1.000 ppm
F2                    -300.13 Hz
PPMCM                 0.60000 ppm/cm
HZCM                180.07800 Hz/cm
```

4-Aryl-2*H*-chromene **3m**: ^{13}C NMR (75MHz, $CDCl_3$)

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Current Data Parameters
NAME                        z
EXPNO                      21
PROCNO                      1

F2 - Acquisition Parameters
Date_               20091029
Time                   80.18
INSTRUM                av300
PROBHD   5 mm DUL 13C-1
PULPROG             zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                       1024
DS                          4
SWH                17980.614 Hz
FIDRES              0.274458 Hz
AQ                  1.8218508 sec
RG                      1448.2
DW                     27.800 usec
DE                      6.00 usec
TE                     296.8 K
D1                  2.00000000 sec
D11                 0.03000000 sec
D12                 0.00002000 sec

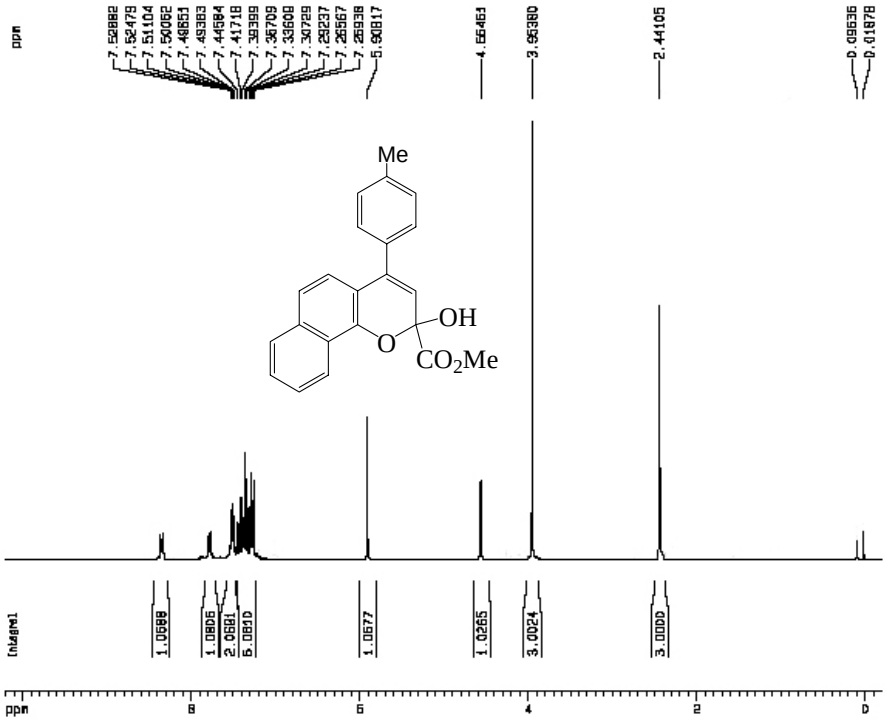
======== CHANNEL f1 ========
NUC1                       13C
P1                      9.80 usec
PL1                     -3.00 dB
SFO1            75.4752953 MHz

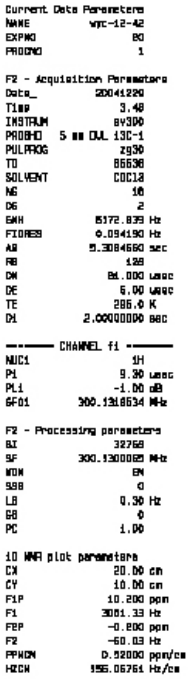
======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                       1H
PCPD2                   80.00 usec
PL2                      0.00 dB
PL12                    17.70 dB
PL13                    17.70 dB
SFO2            300.1312008 MHz

F2 - Processing parameters
SI                      32768
SF                75.4577490 MHz
WDW                        EM
SSB                         0
LB                      1.00 Hz
GB                          0
PC                       1.40

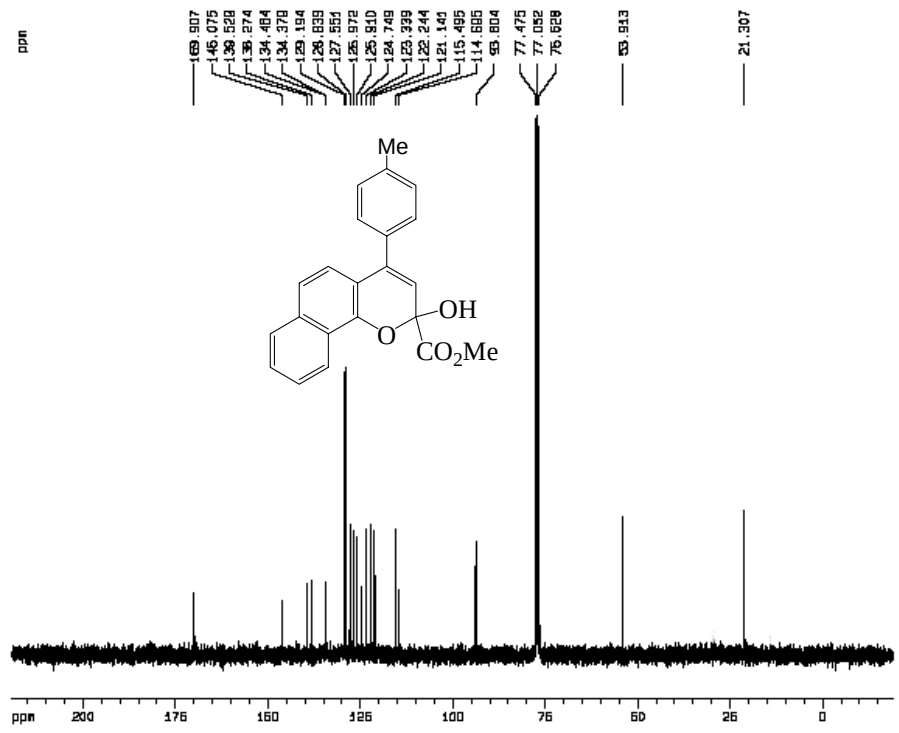
1D NMR plot parameters
CX                      20.00 cm
CY                      12.60 cm
F1P                   218.156 ppm
F1                  16469.16 Hz
F2P                   -19.167 ppm
F2                  -1446.61 Hz
PPMCM                11.91503 ppm/cm
HZCM                899.89008 Hz/cm
```

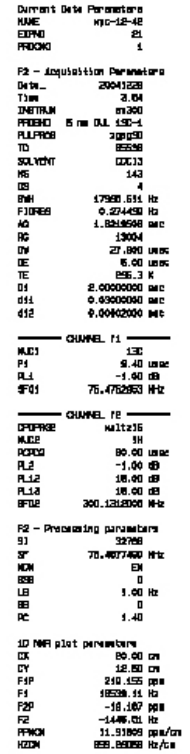
4-Aryl-2*H*-chromene **3n**: ^{1}H NMR (300MHz, $CDCl_3$)



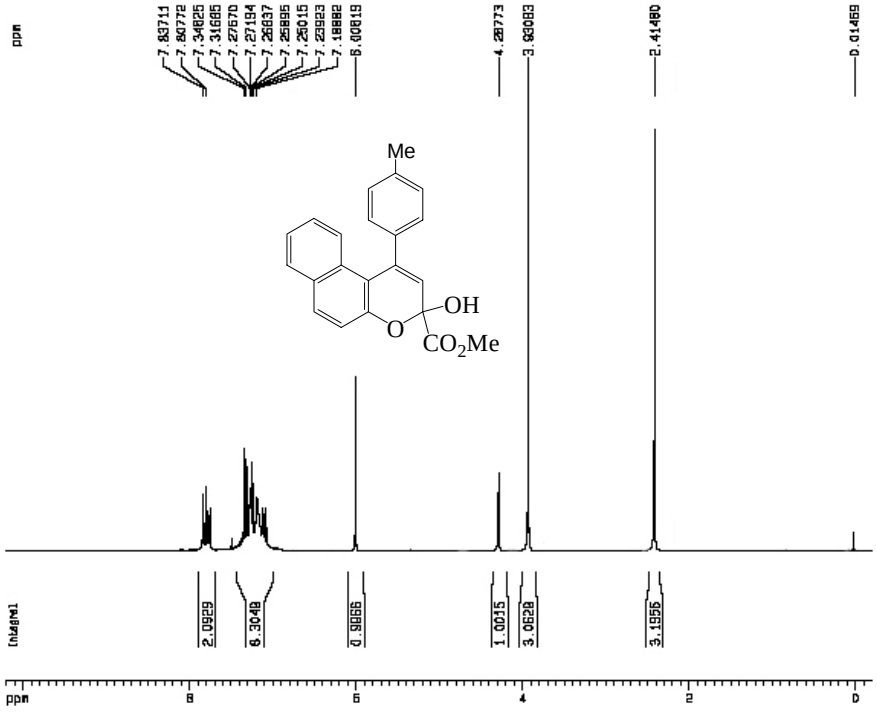


4-Aryl-2*H*-chromene **3n**: ^{13}C NMR (75MHz, $CDCl_3$)





4-Aryl-2*H*-chromene **3o**: ^{1}H NMR (300MHz, $CDCl_3$)




```
Current Data Parameters
NAME            wyc-13-3o
EXPNO                  10
PROCNO                  1

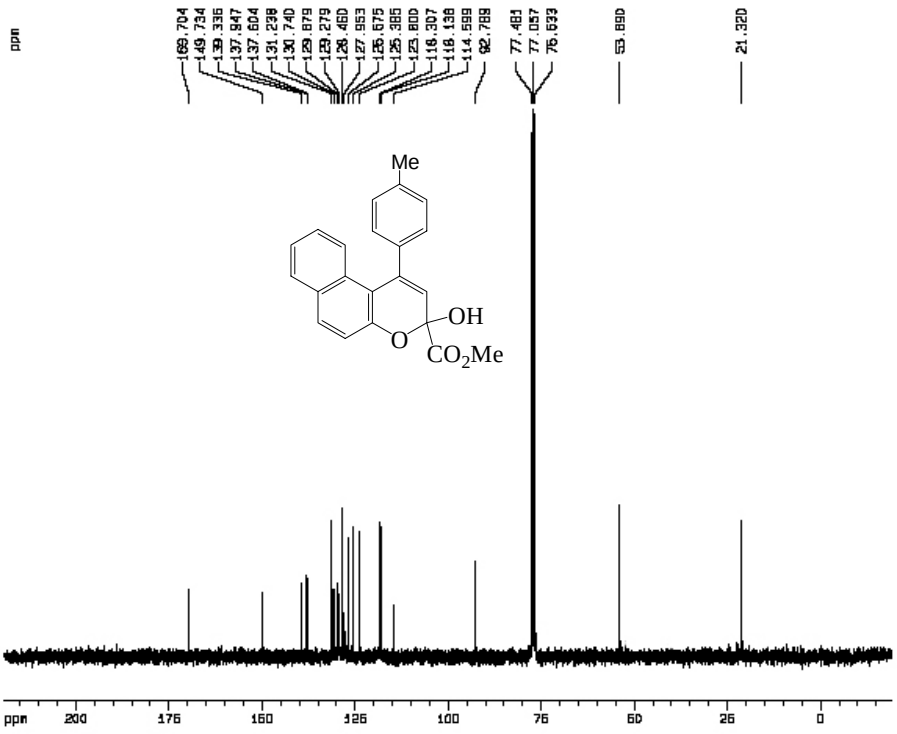
F2 - Acquisition Parameters
Date_          20041224
Time               5.30
INSTRUM          av300
PROBHD  5 mm DUL 13C-1
PULPROG          zg30
TD              65536
SOLVENT          CDCl3
NS                 16
DS                  2
SWH           6172.839 Hz
FIDRES        0.094190 Hz
AQ            5.3084680 sec
RG                203.2
DW               81.000 usec
DE                6.00 usec
TE              296.7 K
D1            2.00000000 sec

======== CHANNEL f1 ========
NUC1                1H
P1                9.30 usec
PL1              -1.00 dB
SFO1        300.1316534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300025 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00

1D NMR plot parameters
CX                20.00 cm
CY                12.60 cm
F1P              10.200 ppm
F1               3061.33 Hz
F2P              -0.800 ppm
F2               -60.03 Hz
PPMCM            0.52000 ppm/cm
HZCM             156.05761 Hz/cm
```

4-Aryl-2*H*-chromene **3o**: ^{13}C NMR (75MHz, $CDCl_3$)




```
Current Data Parameters
NAME            wyc-13-3o
EXPNO                  20
PROCNO                  1

F2 - Acquisition Parameters
Date_          20041227
Time               4.01
INSTRUM          av300
PROBHD  5 mm DUL 13C-1
PULPROG          zgpg30
TD              65536
SOLVENT          CDCl3
NS                 200
DS                   4
SWH           17960.511 Hz
FIDRES        0.274459 Hz
AQ            1.8248598 sec
RG                6792.6
DW               27.800 usec
DE                6.00 usec
TE              298.7 K
D1            2.00000000 sec
d11           0.03000000 sec
d12           0.00002000 sec

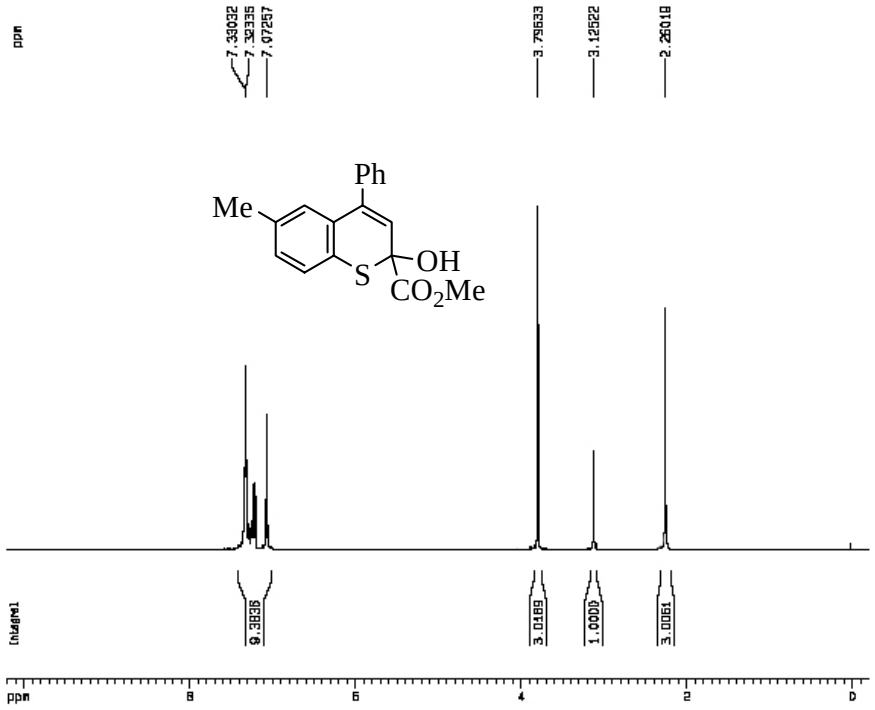
======== CHANNEL f1 ========
NUC1                13C
P1                9.40 usec
PL1              -1.00 dB
SFO1        75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2            80.00 usec
PL2              -1.00 dB
PL12             18.00 dB
PL13             18.00 dB
SFO2        300.1318000 MHz

F2 - Processing parameters
SI                 32768
SF          75.4677480 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40

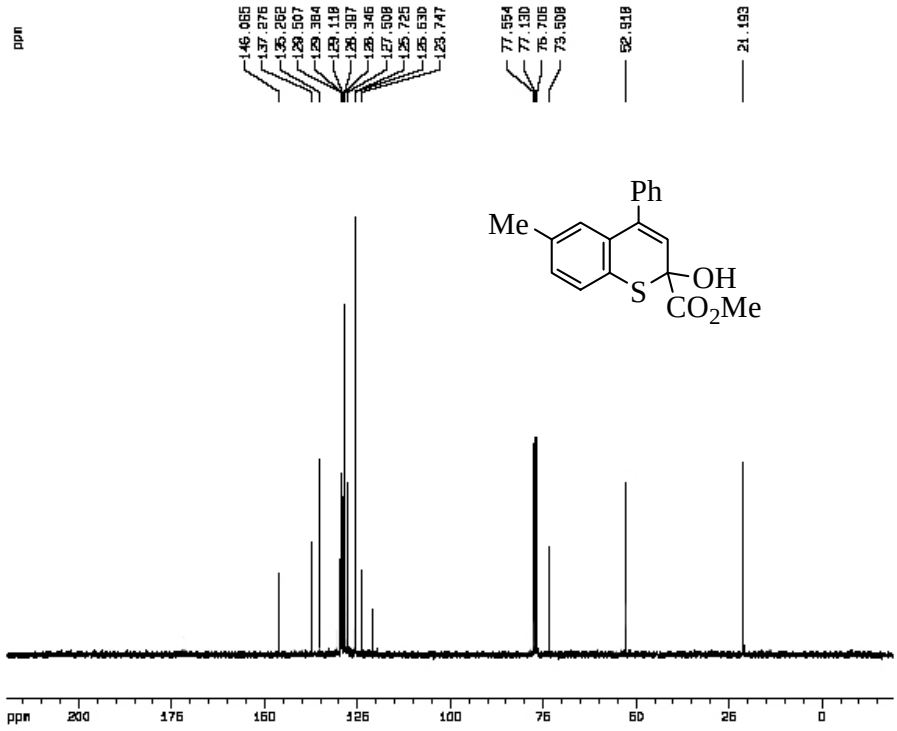
1D NMR plot parameters
CX                20.00 cm
CY                12.60 cm
F1P              249.155 ppm
F1             18538.11 Hz
F2P              -18.187 ppm
F2             -1446.01 Hz
PPMCM            11.91808 ppm/cm
HZCM           888.88068 Hz/cm
```

4-Aryl-2*H*-thiochromene **3p**: ^{1}H NMR (300MHz, $CDCl_3$)



Current Data Parameters
NAME wyc-6-404
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20031112
Time 3.46
INSTRUM av300
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 86536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 80.6
DW 81.000 usec
DE 6.00 usec
TE 282.2 K
D1 2.00000000 sec
CHANNEL f1
NUC1 1H
P1 9.30 usec
PL1 -1.00 dB
SFO1 300.1318634 MHz
F2 - Processing parameters
SI 32768
SF 300.1300025 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
F1P 10.200 ppm
F1 3061.33 Hz
F2P -0.200 ppm
F2 -60.03 Hz
PPMCM 0.52000 ppm/cm
HZCM 156.05761 Hz/cm

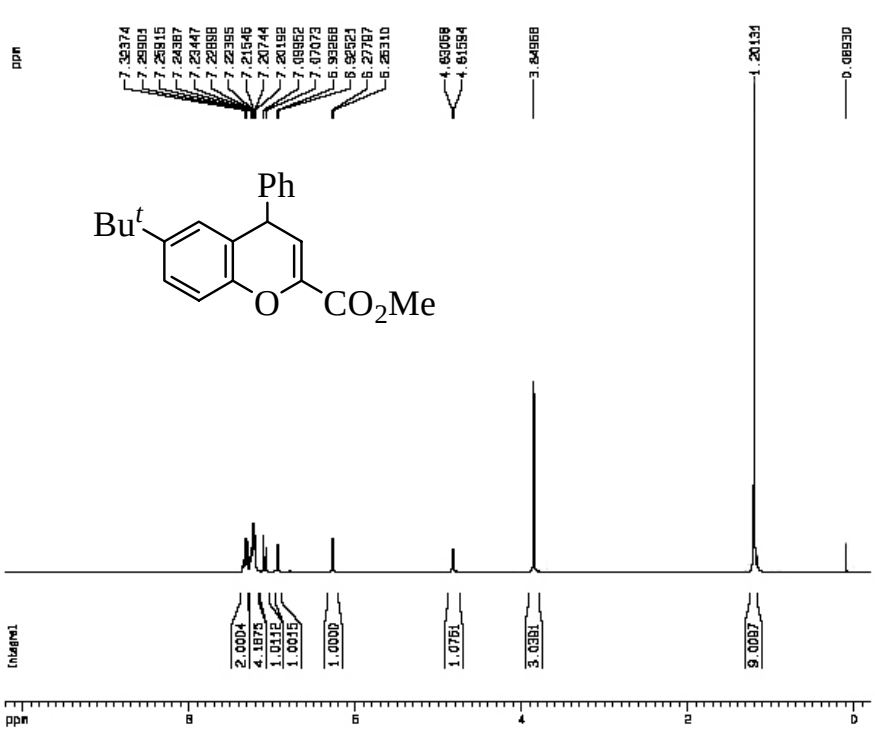
4-Aryl-2*H*-thiochromene **3p**: ^{13}C NMR (75MHz, $CDCl_3$)



Current Data Parameters
NAME wyc-6-404
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20031113
Time 2.41
INSTRUM av300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 300
DS 4
SWH 17985.611 Hz
FIDRES 0.274450 Hz
AQ 1.8249568 sec
RG 256
DW 27.800 usec
DE 6.00 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
CHANNEL f1
NUC1 13C
P1 9.40 usec
PL1 -1.00 dB
SFO1 75.4752853 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 18.00 dB
PL13 18.00 dB
SFO2 300.1318000 MHz
F2 - Processing parameters
SI 32768
SF 75.4677460 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 210.455 ppm
F1 15838.11 Hz
F2P -10.107 ppm
F2 -1446.01 Hz
PPMCM 11.91809 ppm/cm
HZCM 898.86058 Hz/cm

1.2. ^{1}H and ^{13}C NMR spectra of 4*H*-chromene intermediate **13a**

4*H*-chromene intermediate **13a**: ^{1}H NMR (300MHz, $CDCl_3$)




```
Current Data Parameters
NAME            wyc-10-41
EXPNO                  10
PROCNO                  1

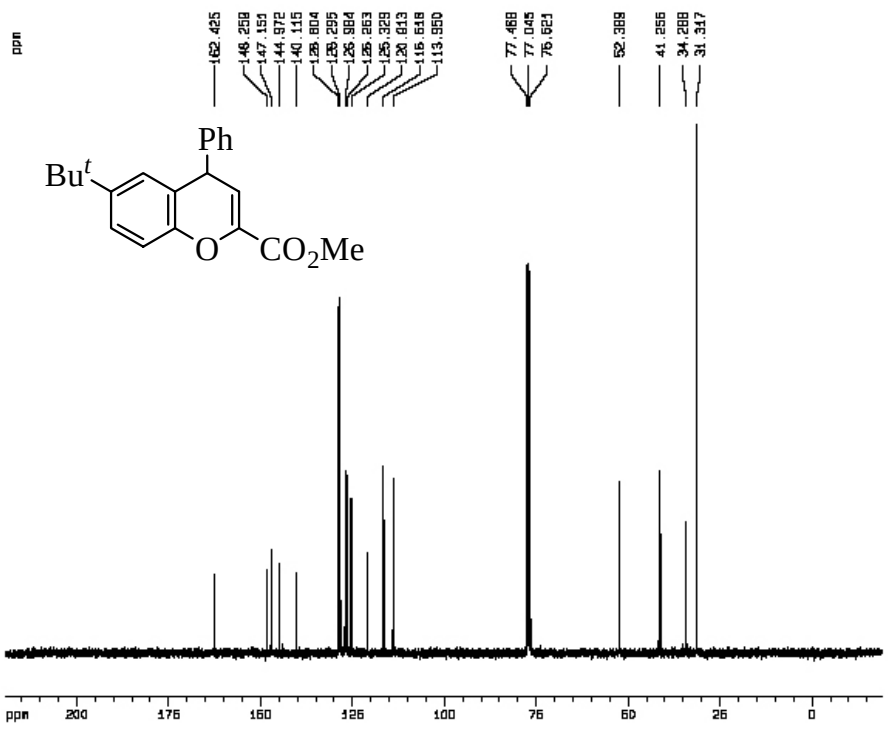
F2 - Acquisition Parameters
Date_          20040630
Time               2.02
INSTRUM           av300
PROBHD  5 mm DUL 13C-1
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH           6172.839 Hz
FIDRES        0.094190 Hz
AQ            5.3084660 sec
RG                 128
DW              81.000 usec
DE               6.00 usec
TE             298.4 K
D1            2.00000000 sec

======== CHANNEL f1 ========
NUC1                1H
P1               9.30 usec
PL1             -1.00 dB
SFO1        300.1318634 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300085 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                 12.60 cm
F1P               10.200 ppm
F1              3061.33 Hz
F2P               -0.800 ppm
F2              -60.03 Hz
PPMCM             9.52000 ppm/cm
HZCM            156.06761 Hz/cm
```

4*H*-chromene intermediate **13a**: ^{13}C NMR (75MHz, $CDCl_3$)




```
Current Data Parameters
NAME            wyc-10-41
EXPNO                  11
PROCNO                  1

F2 - Acquisition Parameters
Date_          20040630
Time               2.08
INSTRUM           spect
PROBHD  5 mm DUL 13C-1
PULPROG          zgpg30
TD               65536
SOLVENT          CDCl3
NS                 428
DS                   4
SWH           17980.691 Hz
FIDRES        0.274459 Hz
AQ            1.8248508 sec
RG                 4096
DW              27.800 usec
DE               6.00 usec
TE             298.8 K
D1            2.00000000 sec
d11           0.03000000 sec
d12           0.00002000 sec

======== CHANNEL f1 ========
NUC1                13C
P1              9.40 usec
PL1             -1.00 dB
SFO1        75.4752853 MHz

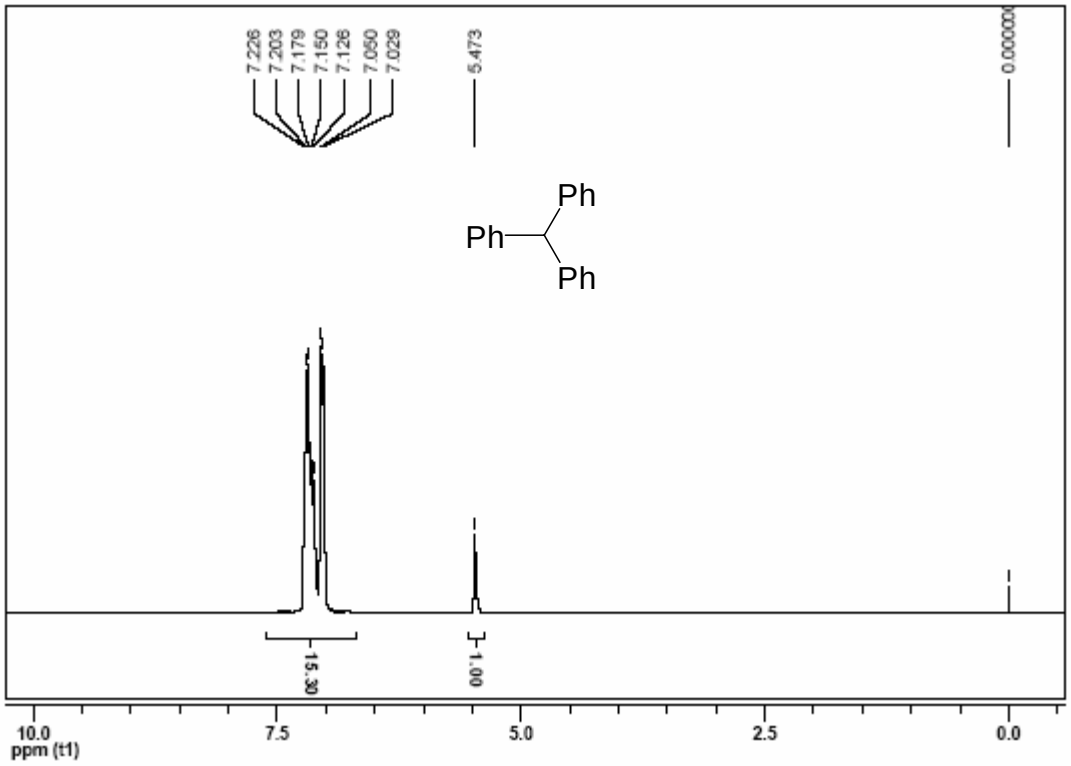
======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2           80.00 usec
PL2             -1.00 dB
PL12            18.00 dB
PL13            18.00 dB
SFO2        300.1318060 MHz

F2 - Processing parameters
SI                 32768
SF          75.4677460 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

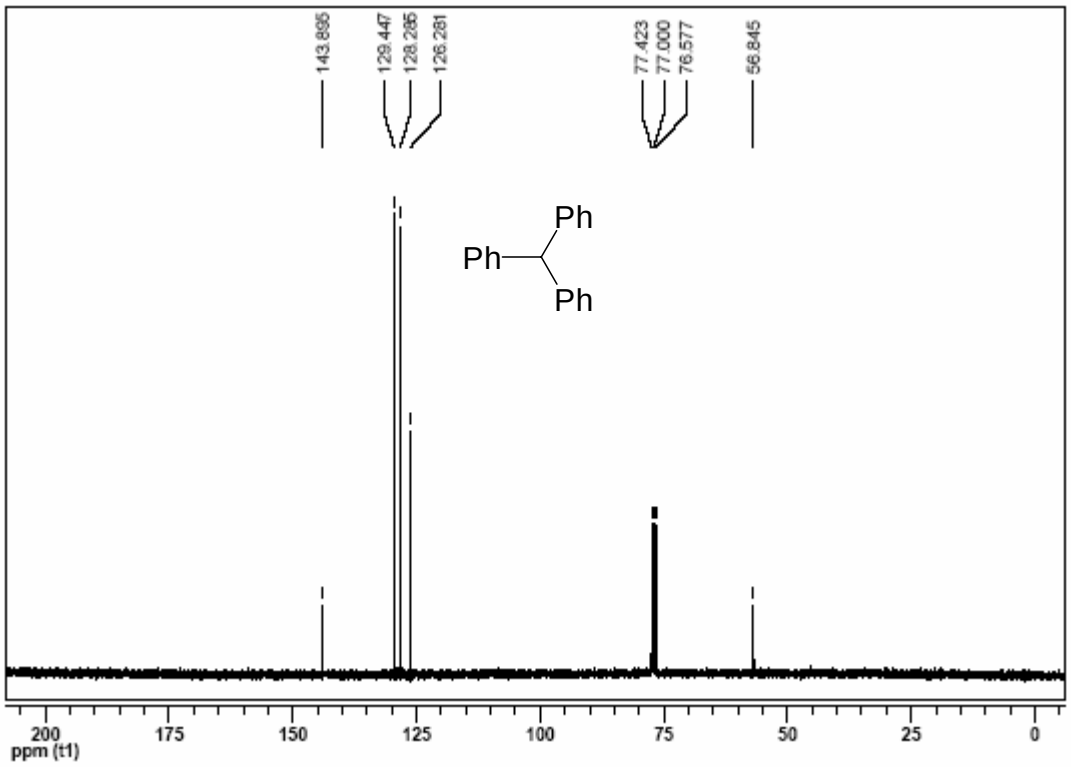
1D NMR plot parameters
CX                 20.00 cm
CY                 12.60 cm
F1P              249.155 ppm
F1             18538.11 Hz
F2P              -18.107 ppm
F2             -1446.01 Hz
PPMCM            11.91869 ppm/cm
HZCM           886.88058 Hz/cm
```

1.3. ^{1}H and ^{13}C NMR spectra of triphenylmethane (**14**)

Triphenylmethane (**14**): ^{1}H NMR (300MHz, $CDCl_3$)

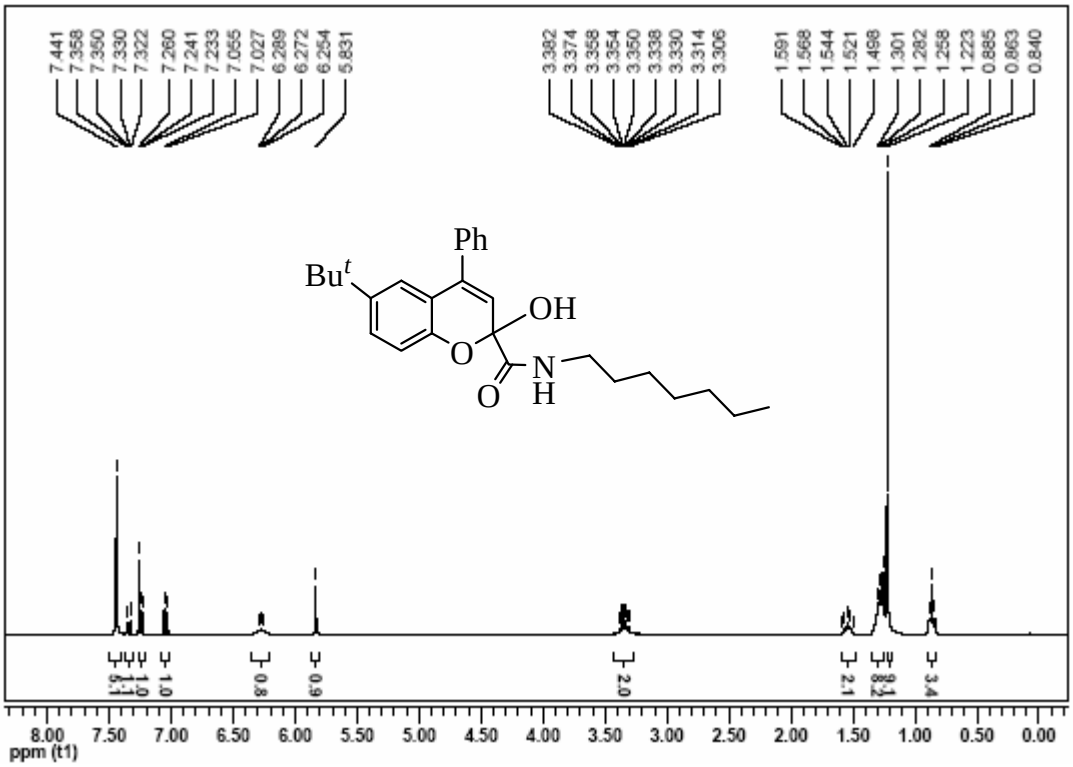


Triphenylmethane (**14**): ^{13}C NMR (75MHz, $CDCl_3$)

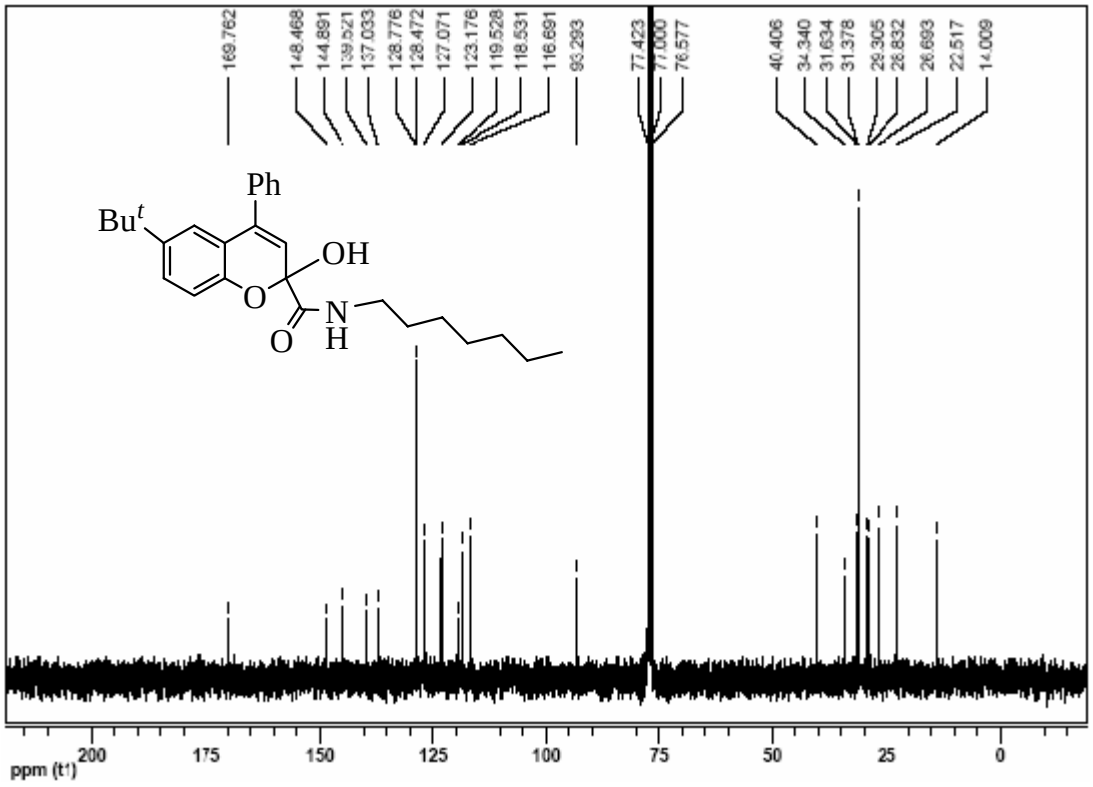


1.4. ^{1}H and ^{13}C NMR spectra of hydroxyl amides **4**

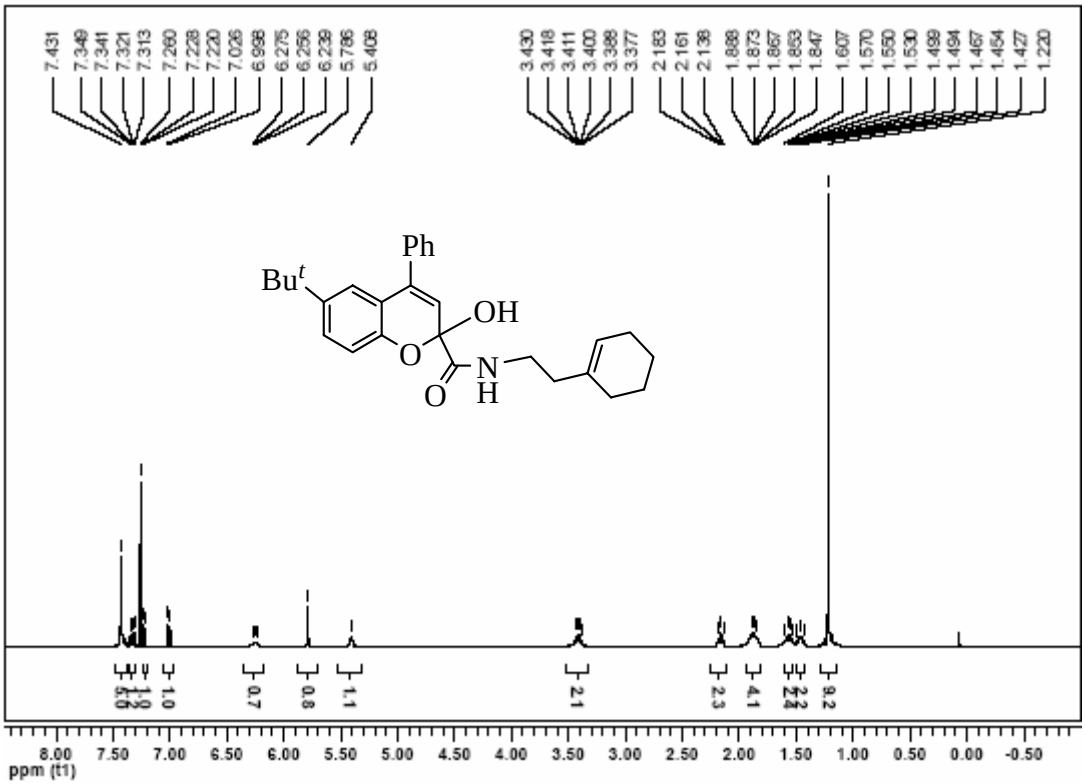
Hydroxyl amide **4a**: ^{1}H NMR (300MHz, $CDCl_3$)



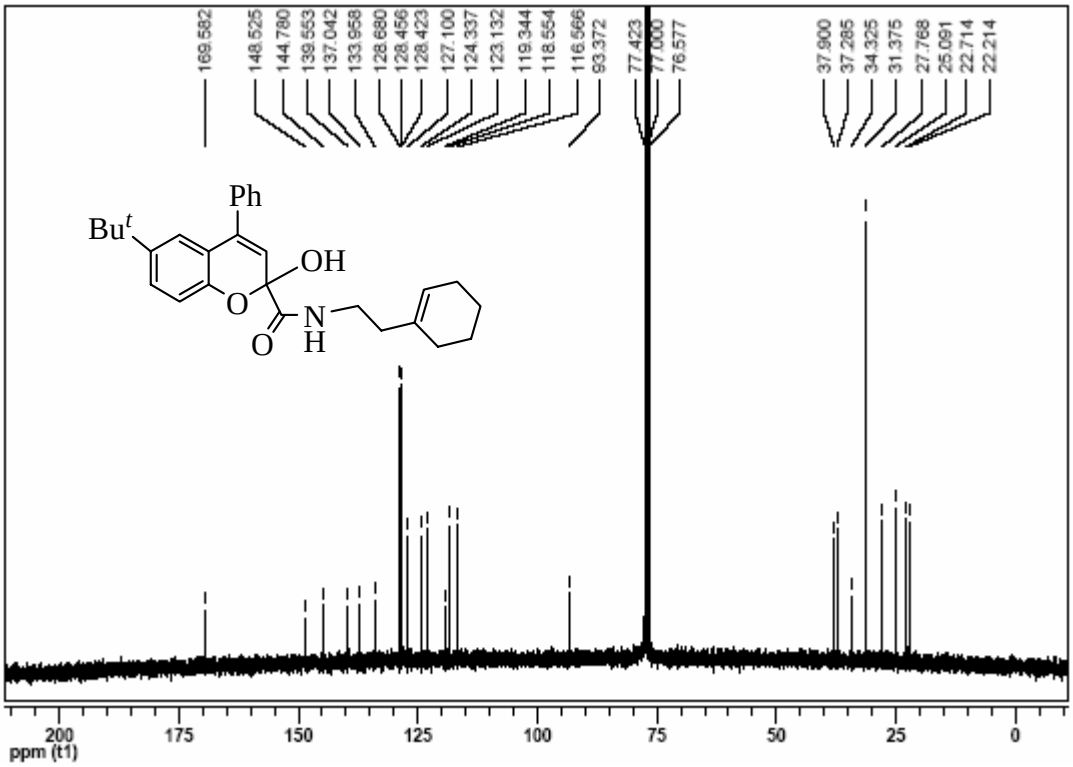
Hydroxyl amide **4a**: ^{13}C NMR (75MHz, $CDCl_3$)



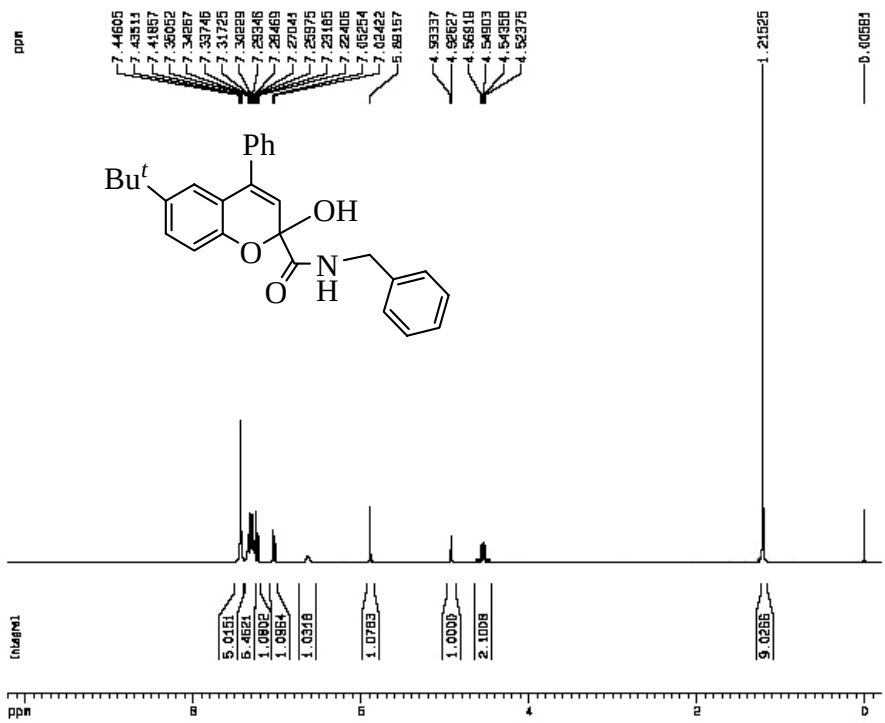
Hydroxyl amide **4b**: ^{1}H NMR (300MHz, $CDCl_3$)



Hydroxyl amide **4b**: ^{13}C NMR (75MHz, $CDCl_3$)



Hydroxyl amide **4c**: ^{1}H NMR (300MHz, $CDCl_3$)

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Current Data Parameters
NAME            wyc-12-10
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_          20041112
Time                3.54
INSTRUM             av300
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 86638
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6172.839 Hz
FIDRES          0.094190 Hz
AQ              5.3084660 sec
RG                   256
DW                 81.000 usec
DE                 6.00 usec
TE                 295.9 K
D1              2.00000000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                 9.30 usec
PL1              -1.00 dB
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                  32768
SF          300.1300000 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                 1.00

1D NMR plot parameters
CX                20.00 cm
CY                12.60 cm
F1P              10.200 ppm
F1               3061.33 Hz
F2P              -0.800 ppm
F2               -60.03 Hz
PPMCM          0.52000 ppm/cm
HZCM           156.06761 Hz/cm
```
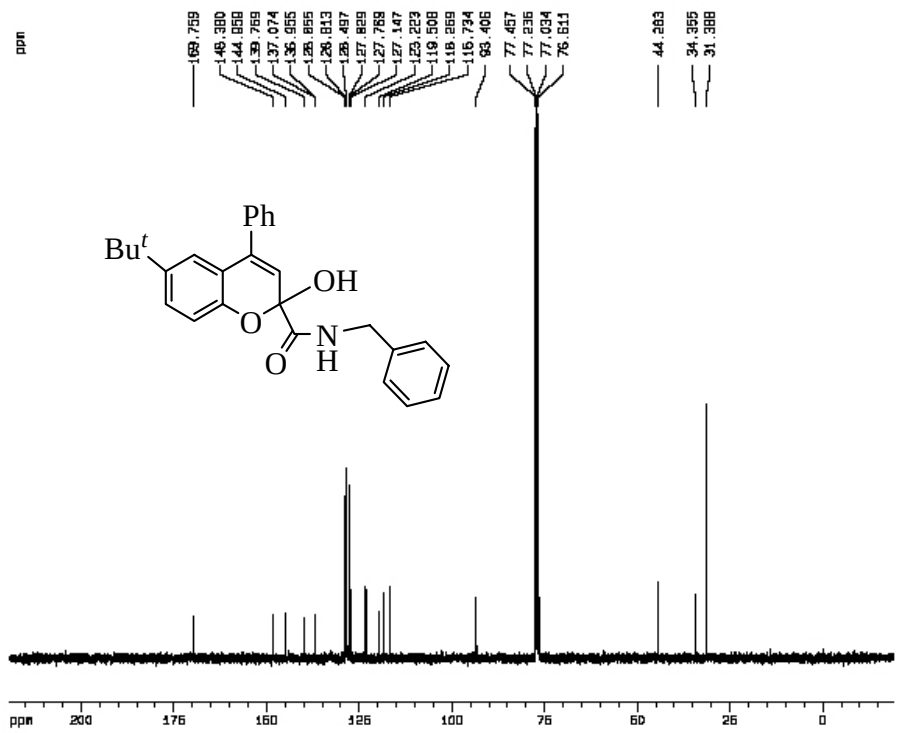
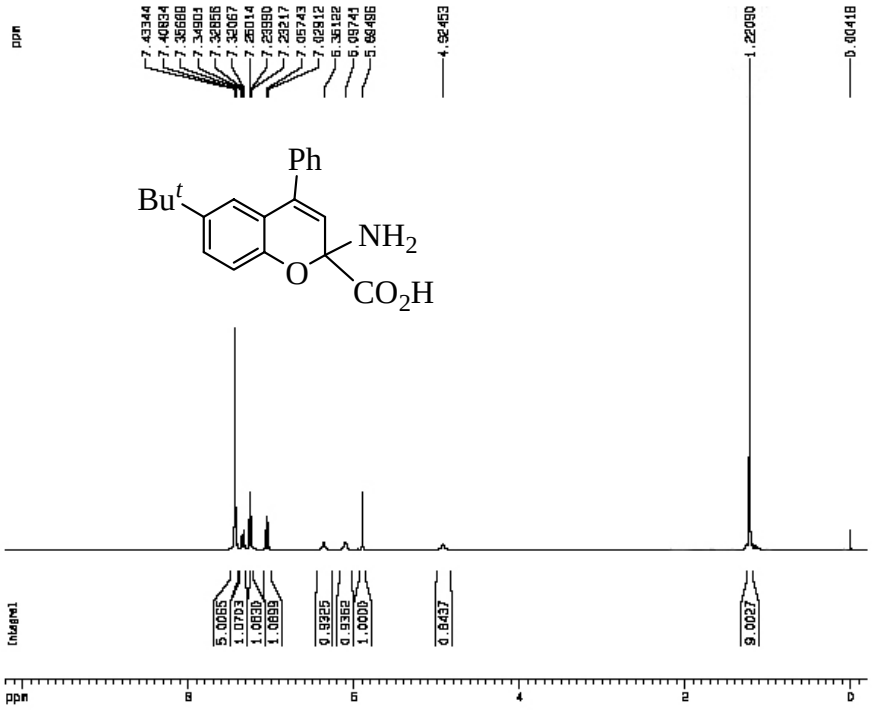

Hydroxyl amide **4c**: ^{13}C NMR (75MHz, $CDCl_3$)




```
Current Data Parameters
NAME            wyc-12-10
EXPNO                  11
PROCNO                  1

F2 - Acquisition Parameters
Date_          20041112
Time                4.28
INSTRUM           av360
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT            CDCl3
NS                   960
DS                     4
SWH            17960.551 Hz
FIDRES          0.274459 Hz
AQ              1.8248598 sec
RG                 812.3
DW                27.800 usec
DE                 6.00 usec
TE                 296.4 K
D1              2.00000000 sec
d11             0.03000000 sec
d12             0.00002000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                 9.40 usec
PL1              -1.00 dB
SFO1        75.4752853 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2              -1.00 dB
PL12             18.00 dB
PL13             18.00 dB
SFO2        300.1318000 MHz

F2 - Processing parameters
SI                  32768
SF          75.4677460 MHz
WDW                    EM
SSB                     0
LB                 1.00 Hz
GB                      0
PC                 1.40

1D NMR plot parameters
CX                20.00 cm
CY                12.60 cm
F1P              210.152 ppm
F1             15838.11 Hz
F2P              -10.187 ppm
F2             -1446.01 Hz
PPMCM          11.51809 ppm/cm
HZCM           868.86058 Hz/cm
```

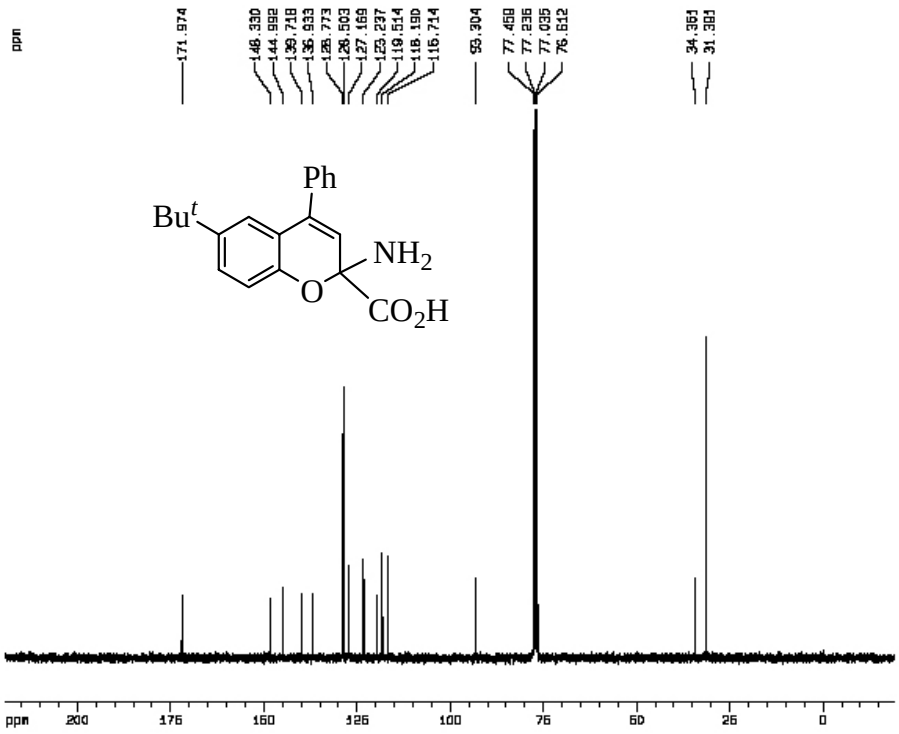
1.5. ^{1}H and ^{13}C NMR spectra of amino acid **5**

Amino acid **5**: ^{1}H NMR (300MHz, $CDCl_3$)




```
Current Data Parameters
NAME            wyc-5-28b
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_           20040405
Time                20.45
INSTRUM             av300
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 86536
SOLVENT            CDCl3
NS                     16
DS                      2
SWH             6172.839 Hz
FIDRES          0.094190 Hz
AQ              5.3084650 sec
RG                  228.1
DW                 81.000 usec
DE                  6.00 usec
TE                297.2 K
D1              2.00000000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                   9.30 usec
PL1                 -1.00 dB
SF01          300.1318634 MHz

F2 - Processing parameters
SI                  32768
SF          300.1300025 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00

1D NMR plot parameters
CX                  20.00 cm
CY                  12.50 cm
F1P                 10.200 ppm
F1                 3061.33 Hz
F2P                -0.800 ppm
F2                 -60.03 Hz
PPMCM               0.52000 ppm/cm
HZCM              156.05761 Hz/cm
```

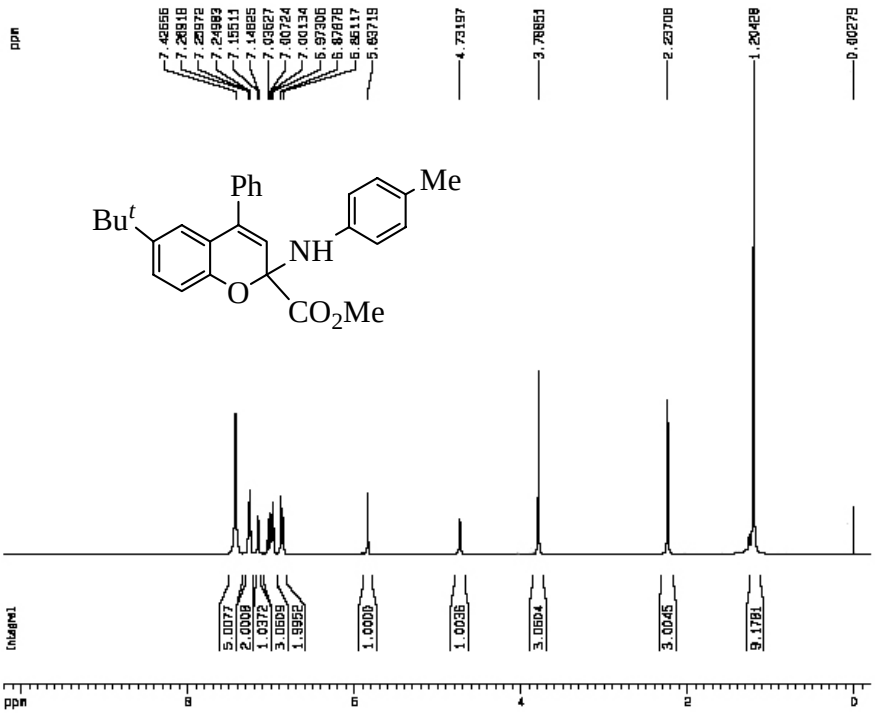
Amino acid **5**: ^{13}C NMR (75MHz, $CDCl_3$)

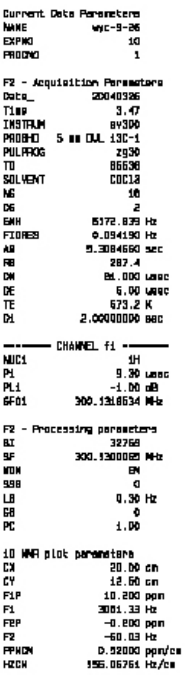



```
Current Data Parameters
NAME            wyc-5-28b
EXPNO                  11
PROCNO                  1

F2 - Acquisition Parameters
Date_           20040406
Time                2.27
INSTRUM             av300
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    587
DS                      4
SWH            17980.611 Hz
FIDRES          0.274459 Hz
AQ              1.8218598 sec
RG                 6080.6
DW                 27.800 usec
DE                  6.00 usec
TE                297.7 K
D1              2.00000000 sec
d11             0.03000000 sec
d12             0.00002000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                   9.40 usec
PL1                 -1.00 dB
SF01          75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                 -1.00 dB
PL12                18.00 dB
PL13                18.00 dB
SF02          300.1318000 MHz

F2 - Processing parameters
SI                  32768
SF          75.4677400 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40

1D NMR plot parameters
CX                  20.00 cm
CY                  12.50 cm
F1P                240.155 ppm
F1              18539.11 Hz
F2P                -18.187 ppm
F2              -1448.01 Hz
PPMCM              11.91809 ppm/cm
HZCM             899.89068 Hz/cm
```

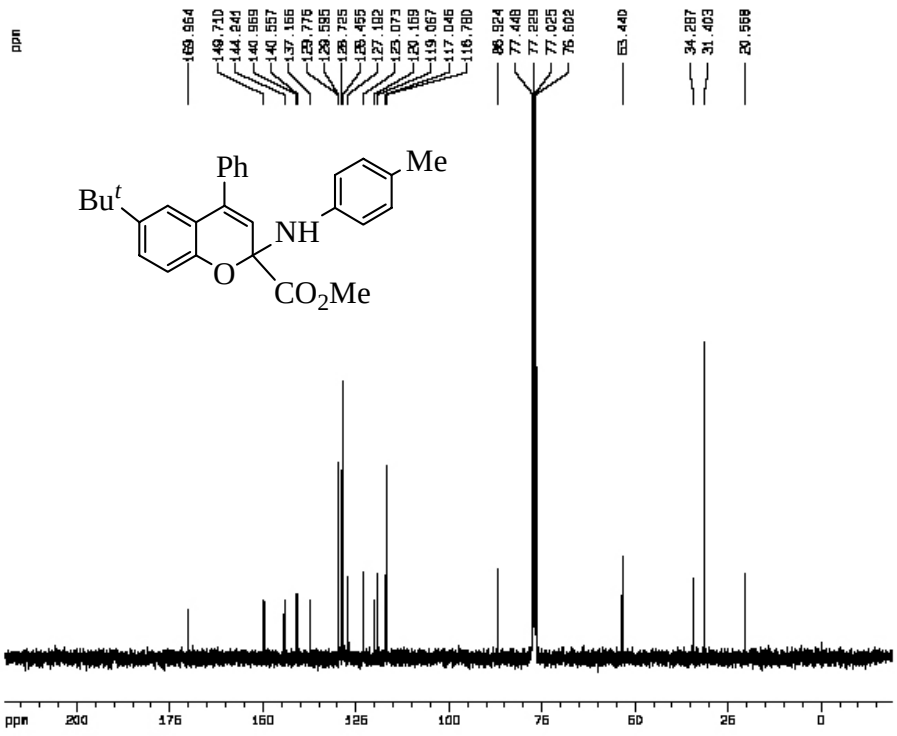
1.6. ^{1}H and ^{13}C NMR spectra of amino esters **6**

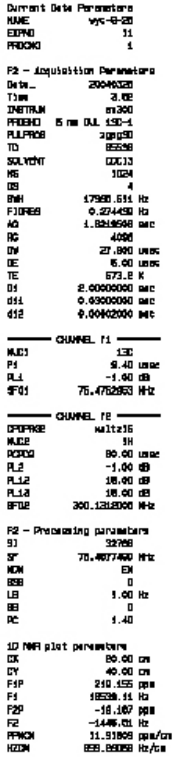
Amino ester **6a**: ^{1}H NMR (300MHz, $CDCl_3$)



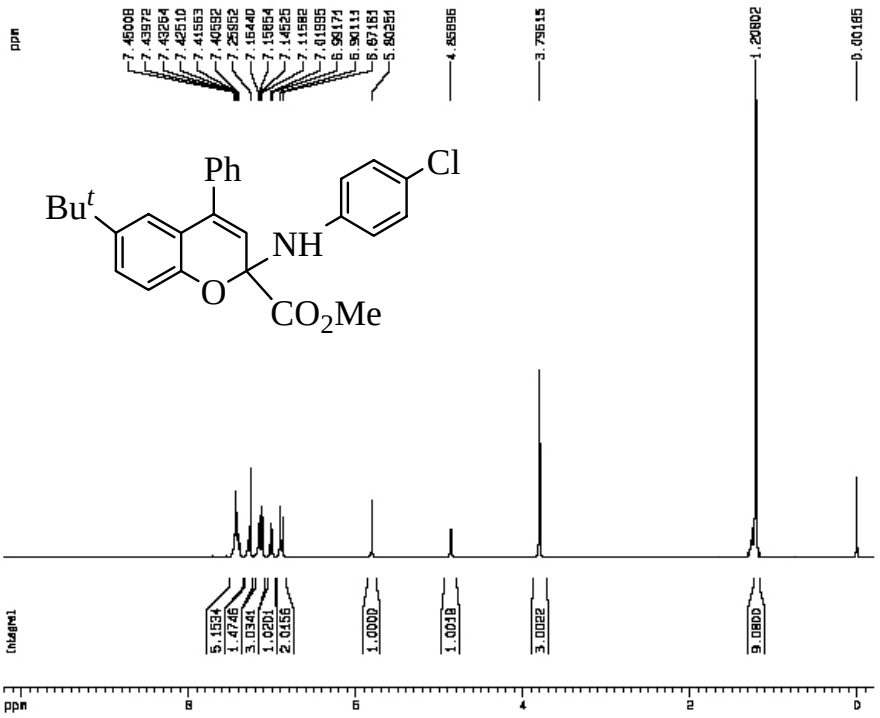


Amino ester **6a**: ^{13}C NMR (75MHz, $CDCl_3$)



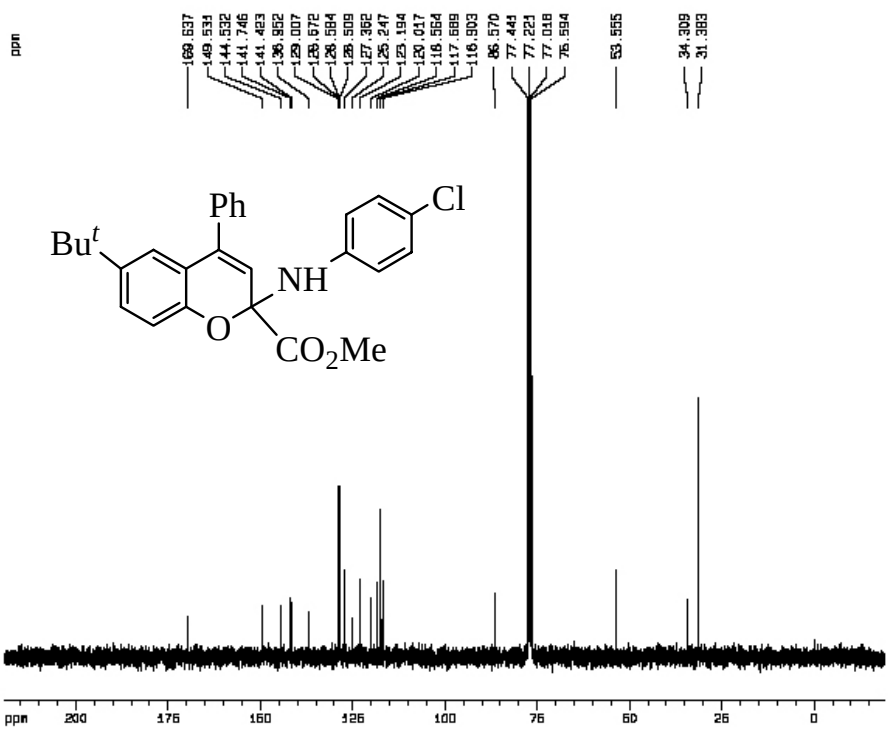


Amino ester **6b**: ^{1}H NMR (300MHz, $CDCl_3$)



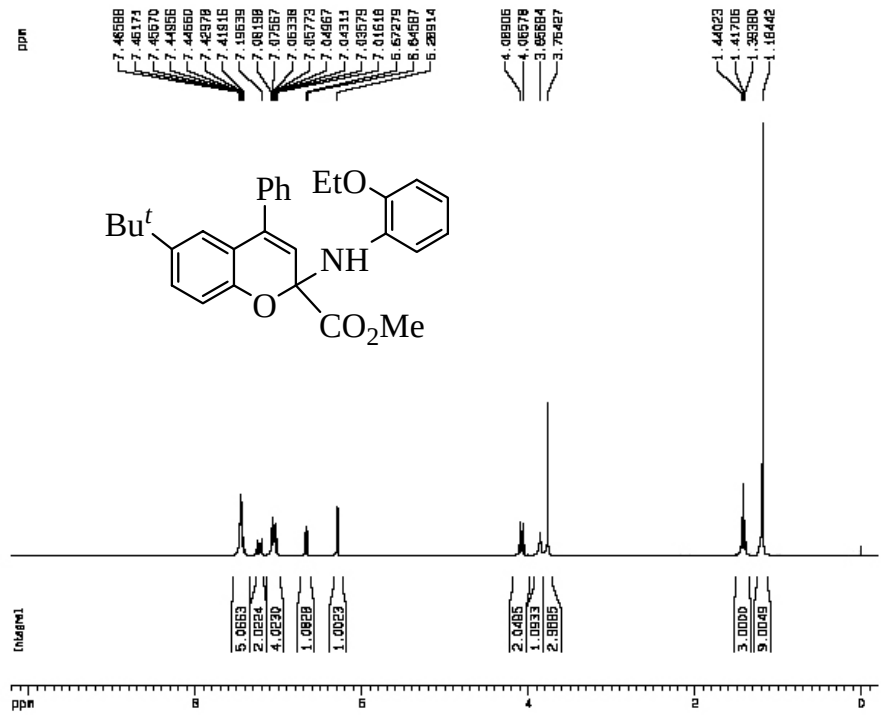

```
Current Data Parameters
NAME                  wyc-12-6
EXPNO                       10
PROCNO                       1

F2 - Acquisition Parameters
Date_               20041110
Time                     21.28
INSTRUM                  av300
PROBHD     5 mm DUL 13C-1
PULPROG                  zg30
TD                      86536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                 6172.839 Hz
FIDRES              0.094190 Hz
AQ                  5.3084660 sec
RG                      322.5
DW                     81.000 usec
DE                      6.00 usec
TE                     295.5 K
D1                  2.00000000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                       9.30 usec
PL1                     -1.00 dB
SFO1            300.1318534 MHz

F2 - Processing parameters
SI                       32768
SF                  300.1300085 MHz
WDW                         EM
SSB                          0
LB                       0.30 Hz
GB                           0
PC                       1.00

1D NMR plot parameters
CX                      20.00 cm
CY                      12.60 cm
F1P                     10.200 ppm
F1                    3061.33 Hz
F2P                    -0.800 ppm
F2                    -60.03 Hz
PPMCM                 0.52000 ppm/cm
HZCM                156.05761 Hz/cm
```

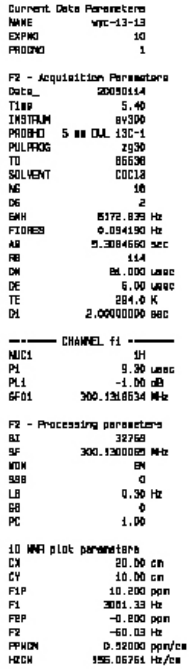
Amino ester **6b**: ^{13}C NMR (75MHz, $CDCl_3$)



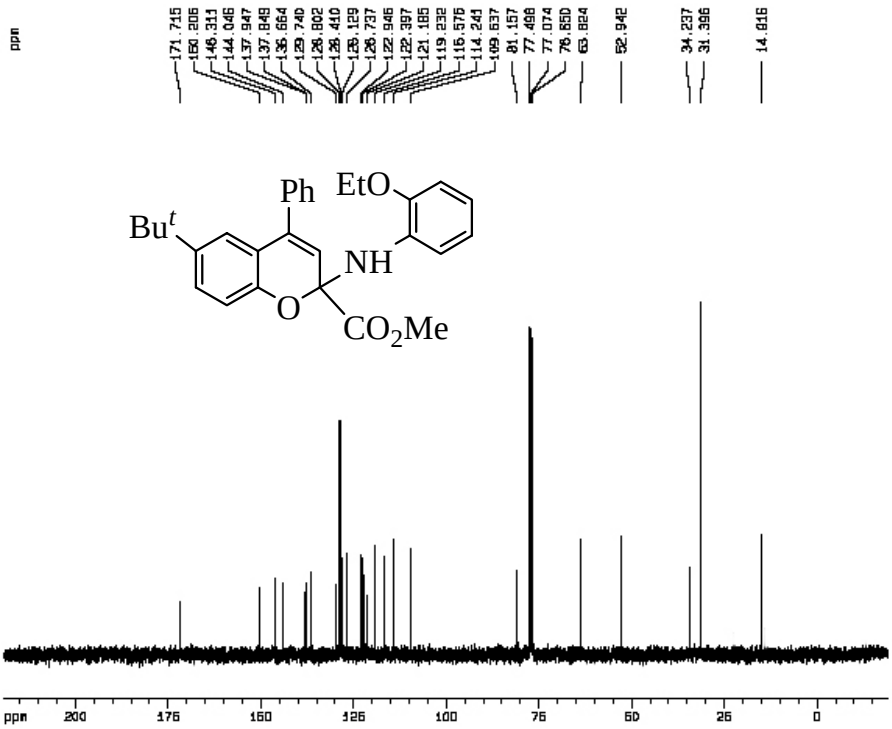

```
Current Data Parameters
NAME                  wyc-12-6
EXPNO                       11
PROCNO                       1

F2 - Acquisition Parameters
Date_               20041118
Time                     15.17
INSTRUM                  av300
PROBHD     5 mm DUL 13C-1
PULPROG                  zgpg30
TD                      65536
SOLVENT                  CDCl3
NS                         783
DS                           4
SWH                 17985.611 Hz
FIDRES              0.274459 Hz
AQ                  1.8249598 sec
RG                      362
DW                     27.800 usec
DE                      6.00 usec
TE                     298.0 K
D1                  2.00000000 sec
d11                 0.03000000 sec
d12                 0.00002000 sec

======== CHANNEL f1 ========
NUC1                       13C
P1                       9.40 usec
PL1                     -1.00 dB
SFO1            75.4752853 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                        1H
PCPD2                   80.00 usec
PL2                     -1.00 dB
PL12                    16.00 dB
PL13                    16.00 dB
SFO2            300.1318060 MHz

F2 - Processing parameters
SI                       32768
SF                  75.4677480 MHz
WDW                         EM
SSB                          0
LB                       1.00 Hz
GB                           0
PC                       1.40

1D NMR plot parameters
CX                      20.00 cm
CY                      25.00 cm
F1P                   240.655 ppm
F1                  18538.11 Hz
F2P                  -18.167 ppm
F2                  -1398.61 Hz
PPMCM                11.91809 ppm/cm
HZCM                 917.88058 Hz/cm
```

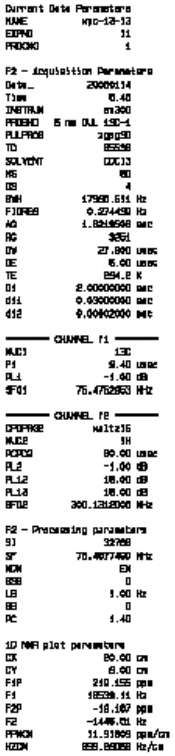
Amino ester **6c**: ^{1}H NMR (300MHz, $CDCl_3$)





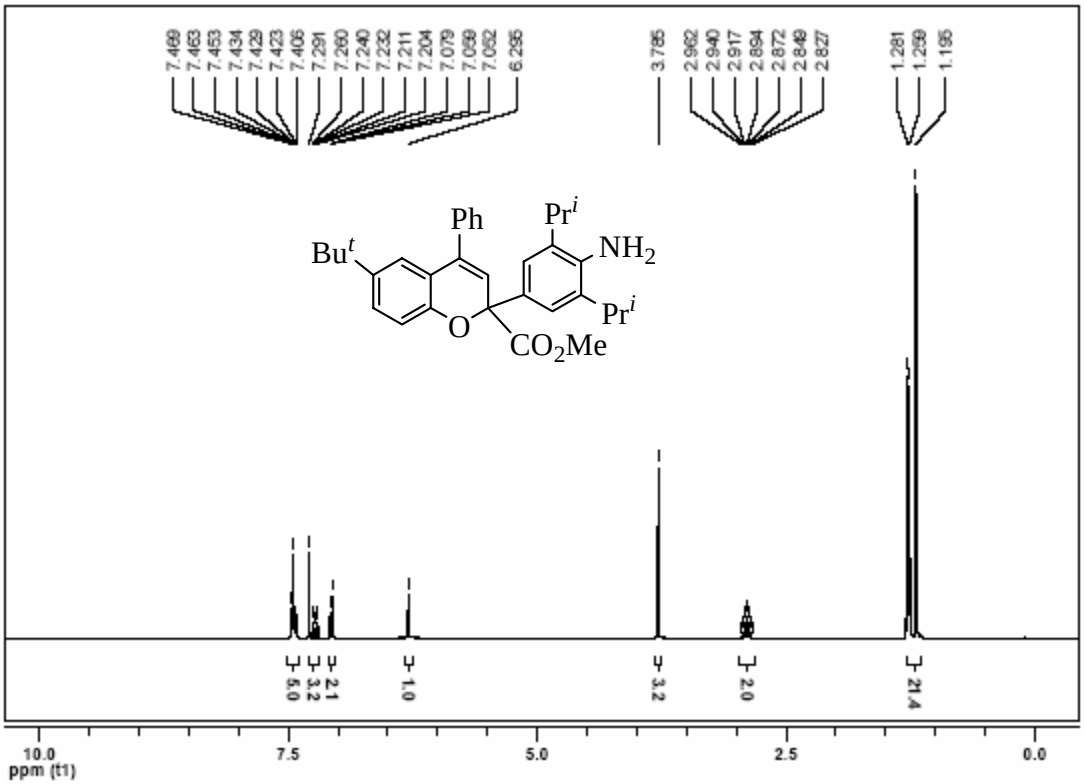
Amino ester **6c**: ^{13}C NMR (75MHz, $CDCl_3$)



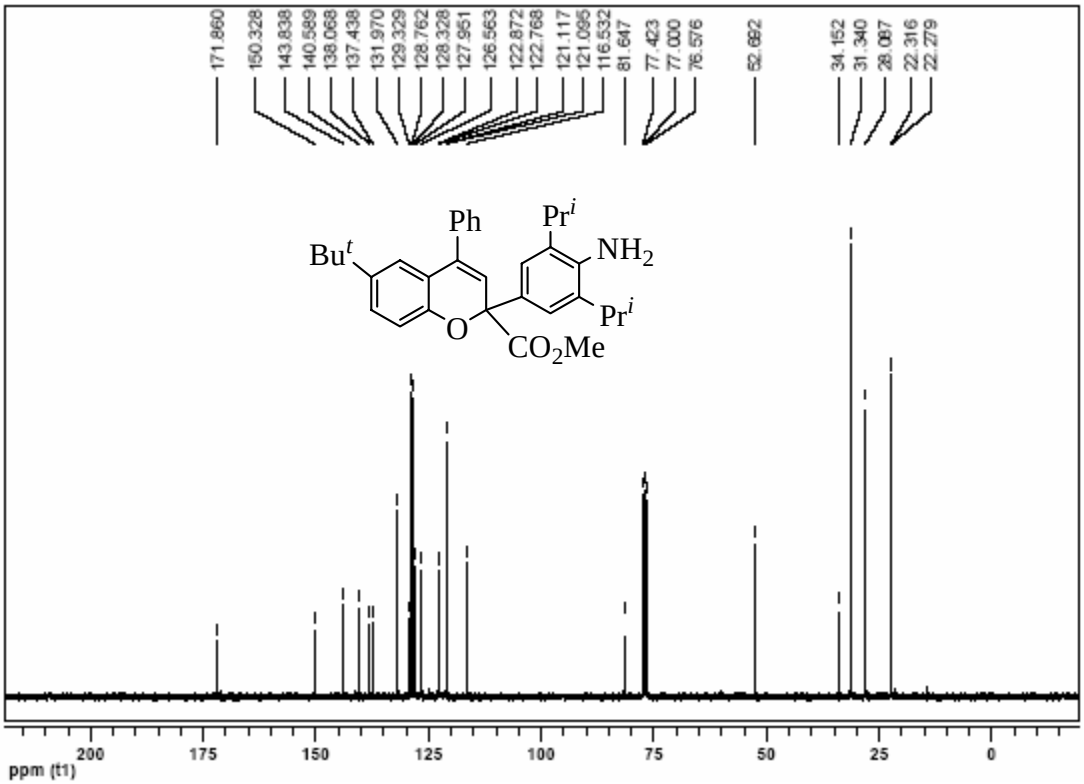


1.7. ^{1}H and ^{13}C NMR spectra of Friedel–Crafts adducts **7**

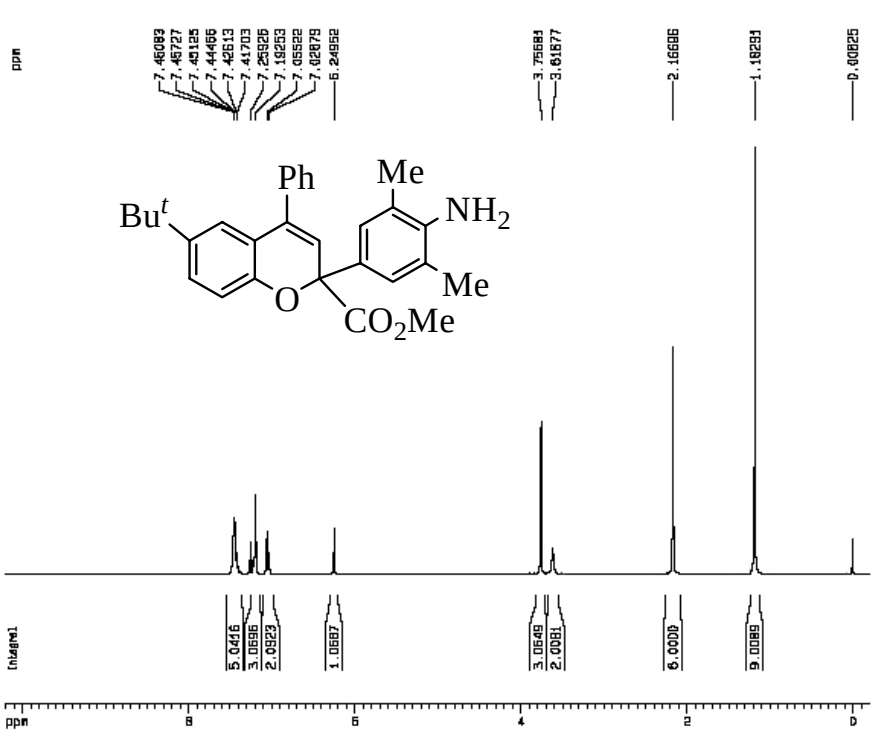
Friedel–Crafts adduct **7a**: ^{1}H NMR (300MHz, $CDCl_3$)



Friedel–Crafts adduct **7a**: ^{13}C NMR (75MHz, $CDCl_3$)



Friedel–Crafts adduct **7b**: ^{1}H NMR (300MHz, $CDCl_3$)



Current Data Parameters
NAME wyc-12-11-2
EXPNO 10
PROCNO 1

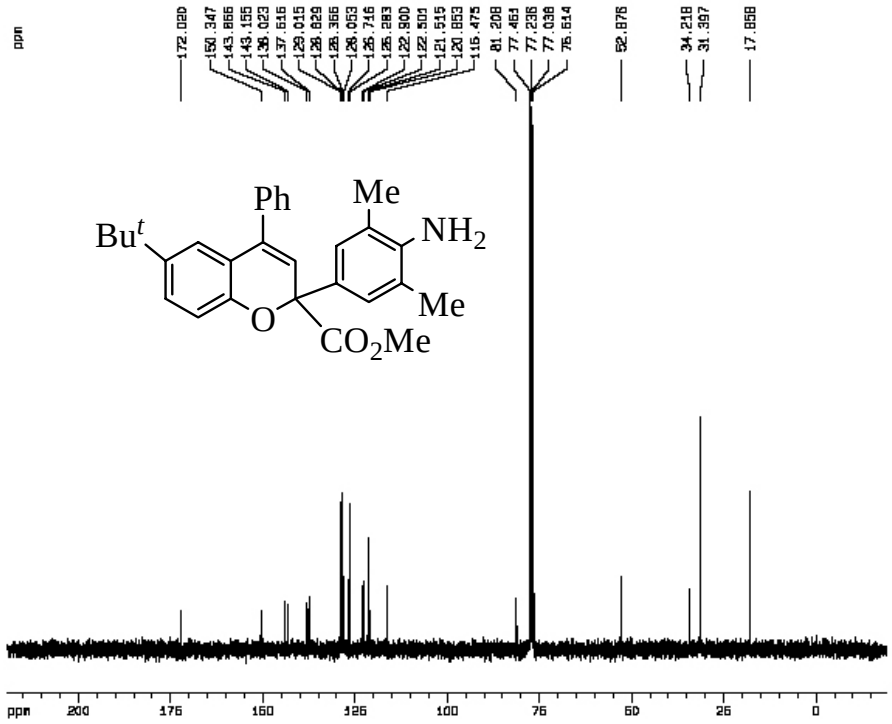
F2 - Acquisition Parameters
Date_ 20041118
Time 21.12
INSTRUM av300
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 296
DW 81.000 usec
DE 6.00 usec
TE 295.5 K
D1 2.00000000 sec

CHANNEL f1
NUC1 1H
P1 9.30 usec
PL1 -1.00 dB
SFO1 300.1318634 MHz

F2 - Processing parameters
SI 32768
SF 300.1300085 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 10.200 ppm
F1 3061.33 Hz
F2P -0.800 ppm
F2 -60.03 Hz
PPMCM 0.52000 ppm/cm
HZCM 155.05761 Hz/cm

Friedel–Crafts adduct **7b**: ^{13}C NMR (75MHz, $CDCl_3$)



Current Data Parameters
NAME wyc-12-11-2
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041118
Time 23.18
INSTRUM av300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 180
DS 4
SWH 17960.514 Hz
FIDRES 0.274459 Hz
AQ 1.8218598 sec
RG 645.1
DW 27.800 usec
DE 6.00 usec
TE 298.8 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

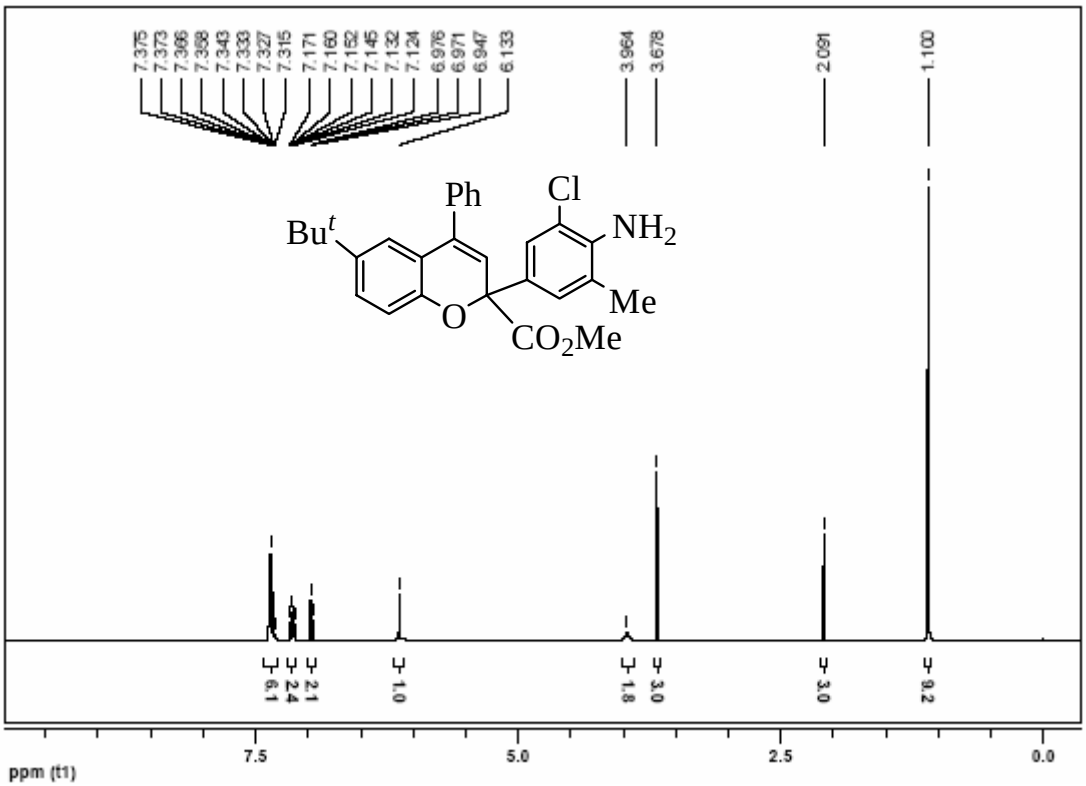
CHANNEL f1
NUC1 13C
P1 9.40 usec
PL1 -1.00 dB
SFO1 75.4752953 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 18.00 dB
PL13 18.00 dB
SFO2 300.1318098 MHz

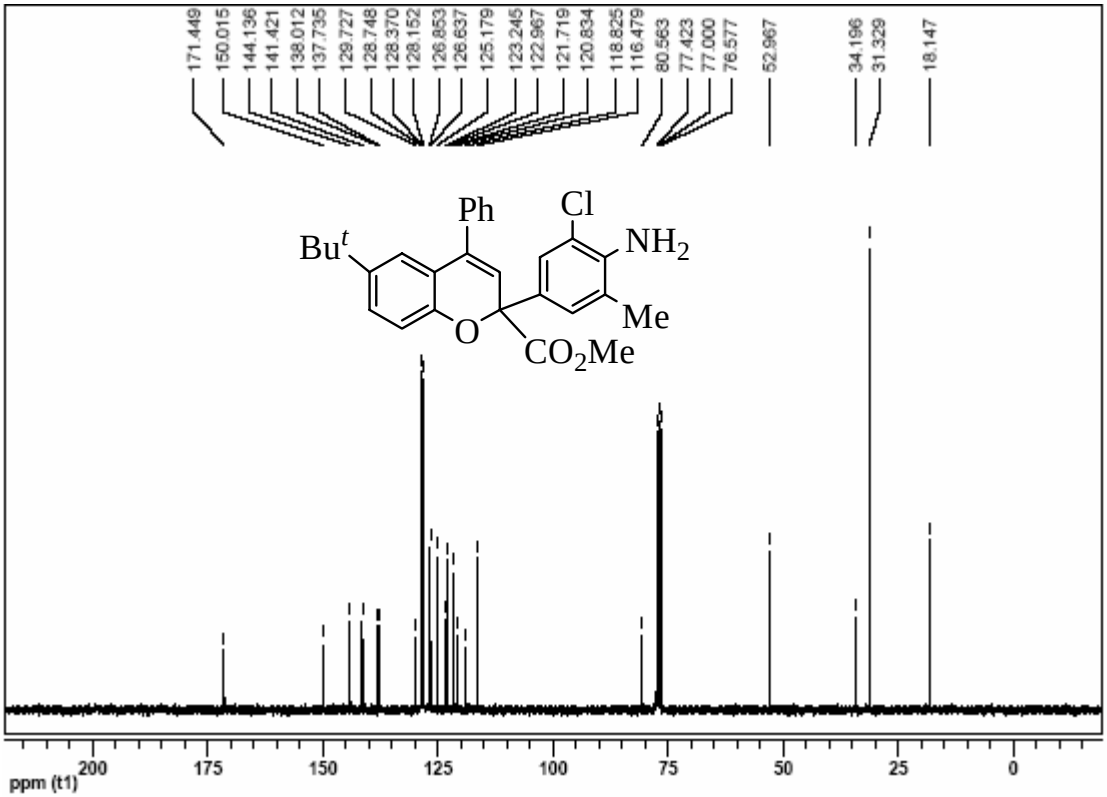
F2 - Processing parameters
SI 32768
SF 75.4677460 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 210.155 ppm
F1 15838.11 Hz
F2P -16.187 ppm
F2 -1446.01 Hz
PPMCM 11.91809 ppm/cm
HZCM 898.86068 Hz/cm

Friedel–Crafts adduct **7c**: ^{1}H NMR (300MHz, $CDCl_3$)

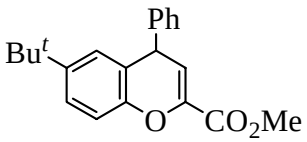


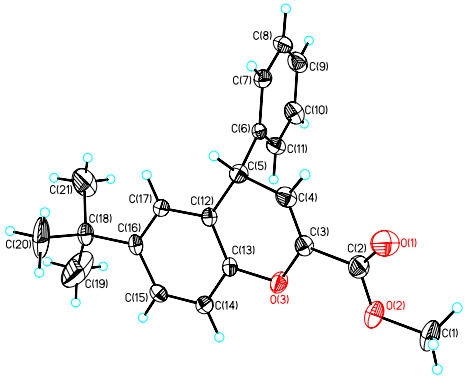
Friedel–Crafts adduct **7c**: ^{13}C NMR (75MHz, $CDCl_3$)



2. Single crystal data

2.1. Single crystal data of 4-aryl-4*H*-chromene intermediate **13a**





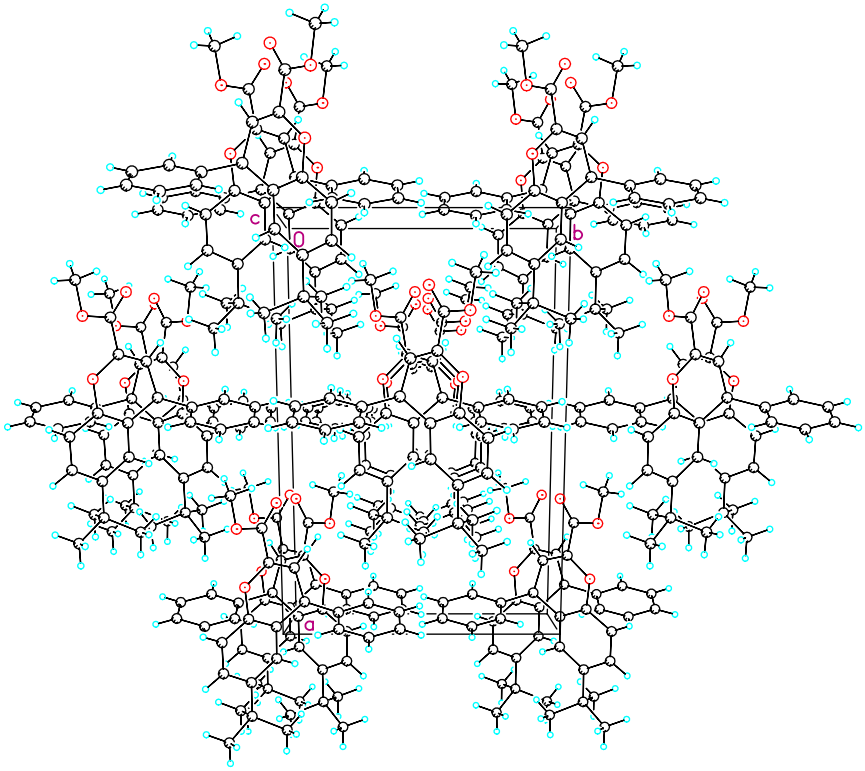


Table 1. Crystal data and structure refinement for **13a**.

Identification code	**13a**
Empirical formula	C21 H22 O3
Formula weight	322.39
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, Cc
Unit cell dimensions	a = 17.683(4) A alpha = 90 deg.
	b = 10.819(2) A beta = 114.81(3) deg.
	c = 10.206(2) A gamma = 90 deg.
Volume	1772.3(6) A^3
Z, Calculated density	4, 1.208 Mg/m^3
Absorption coefficient	0.080 mm^-1
F(000)	688
Crystal size	0.58 x 0.17 x 0.15 mm
Theta range for data collection	2.54 to 27.48 deg.
Limiting indices	0<=h<=22, 0<=k<=14, -13<=l<=11
Reflections collected / unique	6608 / 1990 [R(int) = 0.0799]
Completeness to theta = 27.48	98.0 %
Absorption correction	Empirical
Max. and min. transmission	0.9881 and 0.9551
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1990 / 2 / 217
Goodness-of-fit on F^2	1.017
Final R indices [I>2sigma(I)]	R1 = 0.0698, wR2 = 0.1715
R indices (all data)	R1 = 0.0905, wR2 = 0.1823
Absolute structure parameter	1(2)
Largest diff. peak and hole	0.307 and -0.303 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **13a**.

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	1799(2)	4764(4)	8023(5)	107(2)
O(2)	2393(2)	3433(4)	9860(4)	78(1)
O(3)	3834(2)	3658(3)	9846(3)	61(1)

C(1)	1586(4)	3263(7)	9882(8)	100(2)
C(2)	2401(3)	4274(5)	8902(6)	68(1)
C(3)	3252(2)	4487(4)	8968(4)	50(1)
C(4)	3406(3)	5375(4)	8295(5)	58(1)
C(5)	4257(2)	5725(4)	8478(4)	50(1)
C(6)	4487(2)	6982(3)	9269(5)	45(1)
C(7)	4297(3)	8058(4)	8473(6)	63(1)
C(8)	4477(4)	9184(4)	9216(8)	81(2)
C(9)	4832(3)	9223(5)	10692(7)	78(2)
C(10)	5002(3)	8120(5)	11469(7)	76(1)
C(11)	4833(3)	7036(4)	10754(5)	58(1)
C(12)	4855(2)	4716(3)	9235(4)	44(1)
C(13)	4630(3)	3761(3)	9880(4)	48(1)
C(14)	5178(3)	2826(4)	10614(5)	61(1)
C(15)	5963(3)	2844(4)	10674(6)	61(1)
C(16)	6236(2)	3797(4)	10026(4)	51(1)
C(17)	5664(2)	4702(4)	9322(4)	48(1)
C(18)	7111(3)	3784(5)	10063(5)	65(1)
C(19)	7702(5)	3007(13)	11284(13)	213(7)
C(20)	7072(5)	3278(11)	8667(12)	162(5)
C(21)	7462(5)	5068(7)	10195(14)	155(4)

Table 3. Bond lengths [A] and angles [deg] for **13a**.

O(1)-C(2)	1.192(7)
O(2)-C(2)	1.340(6)
O(2)-C(1)	1.448(6)
O(3)-C(3)	1.375(5)
O(3)-C(13)	1.398(5)
C(2)-C(3)	1.495(6)
C(3)-C(4)	1.275(6)
C(4)-C(5)	1.485(6)
C(5)-C(12)	1.490(6)
C(5)-C(6)	1.546(6)
C(6)-C(11)	1.377(6)
C(6)-C(7)	1.378(5)
C(7)-C(8)	1.399(8)
C(8)-C(9)	1.368(8)

C(9)-C(10)	1.395(8)
C(10)-C(11)	1.347(7)
C(12)-C(13)	1.371(5)
C(12)-C(17)	1.397(5)
C(13)-C(14)	1.384(6)
C(14)-C(15)	1.364(6)
C(15)-C(16)	1.415(6)
C(16)-C(17)	1.375(5)
C(16)-C(18)	1.531(6)
C(18)-C(20)	1.502(10)
C(18)-C(19)	1.503(10)
C(18)-C(21)	1.504(9)

C(2)-O(2)-C(1)	114.3(4)
C(3)-O(3)-C(13)	115.8(3)
O(1)-C(2)-O(2)	124.8(5)
O(1)-C(2)-C(3)	122.0(5)
O(2)-C(2)-C(3)	113.0(4)
C(4)-C(3)-O(3)	124.9(3)
C(4)-C(3)-C(2)	122.0(4)
O(3)-C(3)-C(2)	113.1(4)
C(3)-C(4)-C(5)	123.9(4)
C(4)-C(5)-C(12)	109.9(3)
C(4)-C(5)-C(6)	108.7(3)
C(12)-C(5)-C(6)	113.5(3)
C(11)-C(6)-C(7)	119.9(4)
C(11)-C(6)-C(5)	120.7(3)
C(7)-C(6)-C(5)	119.3(4)
C(6)-C(7)-C(8)	118.2(5)
C(9)-C(8)-C(7)	121.3(5)
C(8)-C(9)-C(10)	119.3(5)
C(11)-C(10)-C(9)	119.4(5)
C(10)-C(11)-C(6)	121.9(4)
C(13)-C(12)-C(17)	117.2(3)
C(13)-C(12)-C(5)	121.0(3)
C(17)-C(12)-C(5)	121.8(3)
C(12)-C(13)-C(14)	122.2(4)
C(12)-C(13)-O(3)	122.7(3)
C(14)-C(13)-O(3)	115.1(3)
C(15)-C(14)-C(13)	118.8(4)
C(14)-C(15)-C(16)	122.0(4)

C(17)-C(16)-C(15)	116.3(3)
C(17)-C(16)-C(18)	122.2(4)
C(15)-C(16)-C(18)	121.4(4)
C(16)-C(17)-C(12)	123.4(4)
C(20)-C(18)-C(19)	108.8(7)
C(20)-C(18)-C(21)	105.9(7)
C(19)-C(18)-C(21)	109.0(8)
C(20)-C(18)-C(16)	109.7(5)
C(19)-C(18)-C(16)	111.7(5)
C(21)-C(18)-C(16)	111.6(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **13a**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

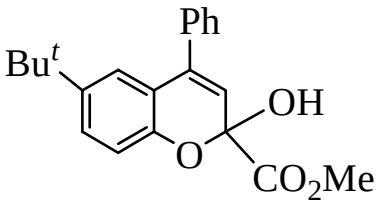
	U11	U22	U33	U23	U13	U12
O(1)	36(2)	97(3)	153(4)	32(3)	7(2)	3(2)
O(2)	47(2)	109(3)	80(2)	-4(2)	31(2)	-10(2)
O(3)	45(2)	79(2)	66(2)	18(2)	29(2)	8(1)
C(1)	59(3)	137(5)	117(5)	-11(4)	51(4)	-16(3)
C(2)	50(3)	67(3)	85(4)	-10(3)	26(3)	-7(2)
C(3)	36(2)	56(2)	49(2)	-6(2)	10(2)	-2(2)
C(4)	40(2)	57(2)	63(3)	2(2)	8(2)	4(2)
C(5)	46(2)	57(2)	43(2)	6(2)	15(2)	3(2)
C(6)	35(2)	43(2)	61(2)	10(2)	24(2)	8(1)
C(7)	52(3)	63(3)	80(3)	21(2)	35(2)	10(2)
C(8)	75(3)	46(2)	138(6)	21(3)	61(4)	13(2)
C(9)	63(3)	55(3)	116(5)	-13(3)	38(3)	-3(2)
C(10)	65(3)	76(4)	78(3)	-14(3)	22(3)	6(2)
C(11)	55(2)	48(2)	64(3)	3(2)	19(2)	3(2)
C(12)	41(2)	49(2)	41(2)	-4(2)	19(2)	1(2)
C(13)	45(2)	52(2)	55(3)	-2(2)	28(2)	4(2)

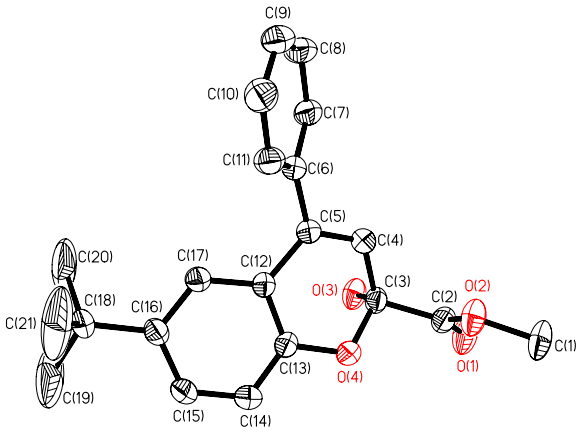
C(14)	59(3)	55(2)	77(3)	13(2)	37(2)	8(2)
C(15)	59(3)	49(2)	78(3)	12(2)	32(2)	18(2)
C(16)	40(2)	62(2)	54(3)	-8(2)	23(2)	7(2)
C(17)	48(2)	47(2)	54(2)	3(2)	26(2)	2(2)
C(18)	43(2)	85(3)	70(3)	-7(3)	26(2)	6(2)
C(19)	59(5)	330(17)	254(14)	170(13)	68(7)	60(7)
C(20)	88(5)	261(12)	176(9)	-89(9)	94(6)	-28(7)
C(21)	74(4)	105(5)	312(14)	-47(7)	105(7)	-27(4)

Table 5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **13a**.

	x	y	z	U(eq)
H(1A)	1628	2651	10590	149
H(1B)	1191	2995	8948	149
H(1C)	1403	4031	10123	149
H(4A)	2959	5832	7652	70
H(5A)	4247	5828	7517	60
H(7A)	4055	8037	7469	75
H(8A)	4354	9919	8697	97
H(9A)	4958	9978	11172	94
H(10A)	5230	8132	12473	91
H(11A)	4952	6303	11278	69
H(14A)	5014	2197	11060	73
H(15A)	6330	2211	11155	73
H(17A)	5825	5339	8880	58
H(19A)	8243	3020	11275	320
H(19B)	7501	2172	11172	320
H(19C)	7741	3332	12185	320
H(20A)	7621	3272	8693	242
H(20B)	6714	3788	7882	242
H(20C)	6857	2451	8532	242
H(21A)	8009	5027	10215	233
H(21B)	7494	5441	11071	233
H(21C)	7106	5555	9384	233

2.2. Single crystal data of 4-aryl-2*H*-chromene **3a**





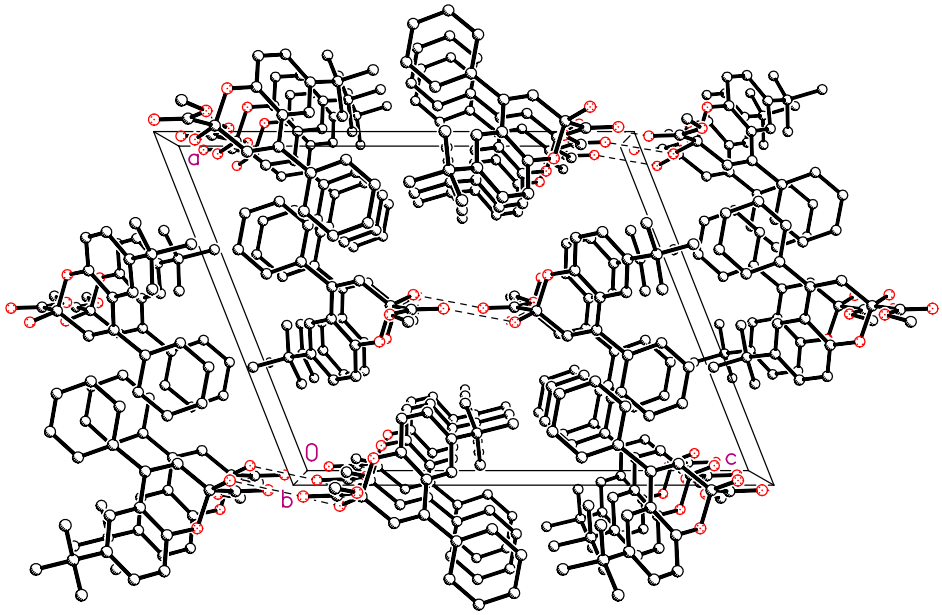


Table 1 Crystal data and structure refinement for **3a**

Identification code	**3a**
Empirical formula	C21 H22 O4
Formula weight	338.39
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	monoclinic, P2(1)/n
Unit cell dimensions	a = 14.3688(8) A alpha = 90 deg.
	b = 7.7163(4) A beta = 111.567(2) deg.
	c = 18.1469(11) A gamma = 90 deg.
Volume	1871.15(18) A^3
Z, Calculated density	4, 1.201 Mg/m^3
Absorption coefficient	0.082 mm^-1
F(000)	720
Crystal size	0.78 x 0.73 x 0.33 mm
Theta range for data collection	2.90 to 27.48 deg.
Limiting indices	0<=h<=18, 0<=k<=10, -23<=l<=21
Reflections collected / unique	3958 / 3958 [R(int) = 0.0000]
Completeness to theta = 27.48	92.3 %
Max. and min. transmission	0.9733 and 0.9382
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3958 / 0 / 227
Goodness-of-fit on F^2	0.673
Final R indices [I>2sigma(I)]	R1 = 0.0521, wR2 = 0.1209
R indices (all data)	R1 = 0.1399, wR2 = 0.1338
Largest diff. peak and hole	0.322 and -0.234 e.A^-3

Table 2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **3a**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	14(2)	6975(3)	417(1)	83(1)
O(2)	176(2)	8291(3)	1540(1)	72(1)
O(3)	-392(1)	3926(2)	955(1)	66(1)
O(4)	938(1)	4988(2)	2023(1)	60(1)
C(1)	354(3)	9936(3)	1217(2)	91(1)
C(2)	38(2)	6941(4)	1077(2)	54(1)
C(3)	-75(2)	5268(3)	1492(2)	50(1)
C(4)	-765(2)	5382(3)	1941(2)	50(1)
C(5)	-615(2)	4436(3)	2584(2)	46(1)
C(6)	-1324(2)	4527(3)	3006(2)	48(1)
C(7)	-2350(2)	4439(4)	2586(2)	64(1)
C(8)	-3012(2)	4705(4)	2977(2)	79(1)
C(9)	-2684(3)	5045(4)	3760(2)	81(1)
C(10)	-1675(3)	5106(4)	4184(2)	75(1)
C(11)	-1005(2)	4833(3)	3809(2)	60(1)
C(12)	298(2)	3381(3)	2882(2)	47(1)
C(13)	1055(2)	3706(3)	2591(2)	52(1)
C(14)	1948(2)	2825(4)	2859(2)	65(1)
C(15)	2080(2)	1497(4)	3401(2)	65(1)
C(16)	1330(2)	1039(4)	3683(2)	53(1)
C(17)	456(2)	2015(3)	3420(2)	52(1)
C(18)	1461(2)	-501(4)	4242(2)	61(1)
C(19)	2255(5)	-1708(7)	4213(4)	272(4)
C(20)	546(3)	-1486(6)	4054(3)	211(3)
C(21)	1772(4)	115(5)	5062(2)	194(3)

Table 3. Bond lengths [A] and angles [deg] for **3a**.

O(1)-C(2)	1.186(3)
O(2)-C(2)	1.307(3)
O(2)-C(1)	1.460(3)
O(3)-C(3)	1.379(3)
O(3)-H(3A)	0.8200
O(4)-C(13)	1.393(3)
O(4)-C(3)	1.436(3)
C(1)-H(1A)	0.9600
C(1)-H(1B)	0.9600
C(1)-H(1C)	0.9600
C(2)-C(3)	1.532(4)
C(3)-C(4)	1.500(3)
C(4)-C(5)	1.325(3)
C(4)-H(4B)	0.9300
C(5)-C(12)	1.468(3)
C(5)-C(6)	1.484(3)
C(6)-C(11)	1.377(3)
C(6)-C(7)	1.390(3)
C(7)-C(8)	1.397(4)
C(7)-H(7A)	0.9300
C(8)-C(9)	1.347(4)
C(8)-H(8A)	0.9300
C(9)-C(10)	1.370(4)
C(9)-H(9A)	0.9300
C(10)-C(11)	1.383(4)
C(10)-H(10A)	0.9300
C(11)-H(11A)	0.9300
C(12)-C(13)	1.395(3)
C(12)-C(17)	1.397(3)
C(13)-C(14)	1.373(3)
C(14)-C(15)	1.384(3)
C(14)-H(14A)	0.9300
C(15)-C(16)	1.397(3)
C(15)-H(15A)	0.9300
C(16)-C(17)	1.390(3)
C(16)-C(18)	1.529(4)
C(17)-H(17A)	0.9300

C(18)-C(20)	1.447(4)
C(18)-C(21)	1.466(4)
C(18)-C(19)	1.489(5)
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
C(20)-H(20A)	0.9600
C(20)-H(20B)	0.9600
C(20)-H(20C)	0.9600
C(21)-H(21A)	0.9600
C(21)-H(21D)	0.9600
C(21)-H(21B)	0.9600

C(2)-O(2)-C(1)	116.3(2)
C(3)-O(3)-H(3A)	109.5
C(13)-O(4)-C(3)	114.84(19)
O(2)-C(1)-H(1A)	109.5
O(2)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
O(2)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
O(1)-C(2)-O(2)	124.9(3)
O(1)-C(2)-C(3)	123.1(3)
O(2)-C(2)-C(3)	112.0(2)
O(3)-C(3)-O(4)	110.6(2)
O(3)-C(3)-C(4)	108.4(2)
O(4)-C(3)-C(4)	110.7(2)
O(3)-C(3)-C(2)	110.6(2)
O(4)-C(3)-C(2)	101.1(2)
C(4)-C(3)-C(2)	115.3(2)
C(5)-C(4)-C(3)	121.3(2)
C(5)-C(4)-H(4B)	119.3
C(3)-C(4)-H(4B)	119.3
C(4)-C(5)-C(12)	117.6(2)
C(4)-C(5)-C(6)	120.6(2)
C(12)-C(5)-C(6)	121.7(2)
C(11)-C(6)-C(7)	117.6(3)
C(11)-C(6)-C(5)	122.0(2)
C(7)-C(6)-C(5)	120.3(3)
C(6)-C(7)-C(8)	119.8(3)

C(6)-C(7)-H(7A)	120.1
C(8)-C(7)-H(7A)	120.1
C(9)-C(8)-C(7)	121.7(3)
C(9)-C(8)-H(8A)	119.2
C(7)-C(8)-H(8A)	119.2
C(8)-C(9)-C(10)	119.1(3)
C(8)-C(9)-H(9A)	120.4
C(10)-C(9)-H(9A)	120.4
C(9)-C(10)-C(11)	120.2(3)
C(9)-C(10)-H(10A)	119.9
C(11)-C(10)-H(10A)	119.9
C(6)-C(11)-C(10)	121.6(3)
C(6)-C(11)-H(11A)	119.2
C(10)-C(11)-H(11A)	119.2
C(13)-C(12)-C(17)	116.8(2)
C(13)-C(12)-C(5)	118.5(2)
C(17)-C(12)-C(5)	124.7(2)
C(14)-C(13)-O(4)	117.2(2)
C(14)-C(13)-C(12)	122.3(3)
O(4)-C(13)-C(12)	120.6(2)
C(13)-C(14)-C(15)	119.0(3)
C(13)-C(14)-H(14A)	120.5
C(15)-C(14)-H(14A)	120.5
C(14)-C(15)-C(16)	121.7(3)
C(14)-C(15)-H(15A)	119.2
C(16)-C(15)-H(15A)	119.2
C(17)-C(16)-C(15)	117.3(3)
C(17)-C(16)-C(18)	121.6(3)
C(15)-C(16)-C(18)	121.1(2)
C(16)-C(17)-C(12)	122.8(3)
C(16)-C(17)-H(17A)	118.6
C(12)-C(17)-H(17A)	118.6
C(20)-C(18)-C(21)	108.7(4)
C(20)-C(18)-C(19)	107.7(4)
C(21)-C(18)-C(19)	106.7(4)
C(20)-C(18)-C(16)	111.9(3)
C(21)-C(18)-C(16)	109.8(3)
C(19)-C(18)-C(16)	111.8(3)
C(18)-C(19)-H(19A)	109.5
C(18)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5

C(18)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(18)-C(20)-H(20A)	109.5
C(18)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(18)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(18)-C(21)-H(21A)	109.5
C(18)-C(21)-H(21D)	109.5
H(21A)-C(21)-H(21D)	109.5
C(18)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
H(21D)-C(21)-H(21B)	109.5

Symmetry transformations used to generate equivalent atoms:

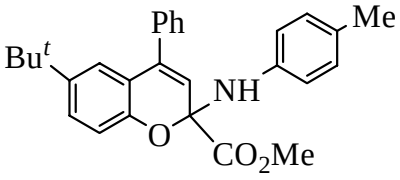
Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **3a**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

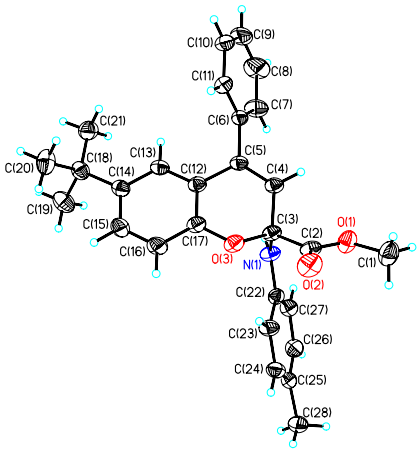
	U11	U22	U33	U23	U13	U12
O(1)	139(2)	61(1)	60(1)	7(1)	52(1)	-6(1)
O(2)	110(2)	45(1)	65(1)	-1(1)	38(1)	-7(1)
O(3)	96(2)	49(1)	66(1)	-1(1)	42(1)	-6(1)
O(4)	51(1)	64(1)	69(1)	20(1)	28(1)	4(1)
C(1)	124(3)	42(2)	110(3)	11(2)	48(2)	-13(2)
C(2)	58(2)	49(2)	59(2)	3(2)	26(2)	-3(2)
C(3)	58(2)	44(2)	47(2)	4(2)	20(2)	0(2)
C(4)	47(2)	50(2)	51(2)	2(2)	18(1)	3(1)
C(5)	44(2)	47(2)	49(2)	0(2)	18(1)	-1(1)
C(6)	42(2)	48(2)	53(2)	7(1)	18(1)	2(1)
C(7)	49(2)	73(2)	68(2)	12(2)	21(2)	-2(2)
C(8)	48(2)	103(3)	90(3)	20(2)	30(2)	2(2)
C(9)	69(2)	100(3)	87(3)	21(2)	45(2)	13(2)
C(10)	88(2)	81(2)	64(2)	5(2)	36(2)	8(2)
C(11)	53(2)	72(2)	60(2)	3(2)	25(2)	1(2)
C(12)	46(2)	46(2)	47(2)	5(1)	16(1)	1(1)
C(13)	53(2)	49(2)	55(2)	8(2)	21(2)	-3(2)
C(14)	48(2)	72(2)	78(2)	14(2)	27(2)	6(2)
C(15)	53(2)	68(2)	76(2)	17(2)	28(2)	18(2)
C(16)	49(2)	55(2)	53(2)	7(2)	15(1)	9(2)
C(17)	51(2)	56(2)	53(2)	6(2)	24(1)	5(2)
C(18)	60(2)	61(2)	58(2)	19(2)	17(2)	11(2)
C(19)	391(9)	183(5)	397(9)	218(6)	329(8)	217(6)
C(20)	134(4)	155(4)	243(6)	148(4)	-49(4)	-71(4)
C(21)	314(7)	137(4)	65(3)	42(3)	-7(4)	-62(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **3a**.

	x	y	z	U(eq)
H(3A)	-143	4030	617	100
H(1A)	444	10837	1602	136
H(1B)	-209	10209	746	136
H(1C)	945	9845	1091	136
H(4B)	-1309	6132	1765	60
H(7A)	-2594	4204	2045	76
H(8A)	-3697	4645	2691	95
H(9A)	-3137	5236	4009	97
H(10A)	-1439	5333	4725	90
H(11A)	-322	4856	4107	72
H(14A)	2456	3115	2679	78
H(15A)	2682	895	3582	78
H(17A)	-46	1747	3610	62
H(19A)	2312	-2661	4567	408
H(19B)	2882	-1104	4369	408
H(19C)	2082	-2139	3683	408
H(20A)	655	-2432	4420	317
H(20B)	347	-1930	3525	317
H(20C)	28	-749	4094	317
H(21A)	1842	-855	5409	291
H(21D)	1276	896	5108	291
H(21B)	2401	708	5204	291

2.3. Single crystal data of amino ester **6a**





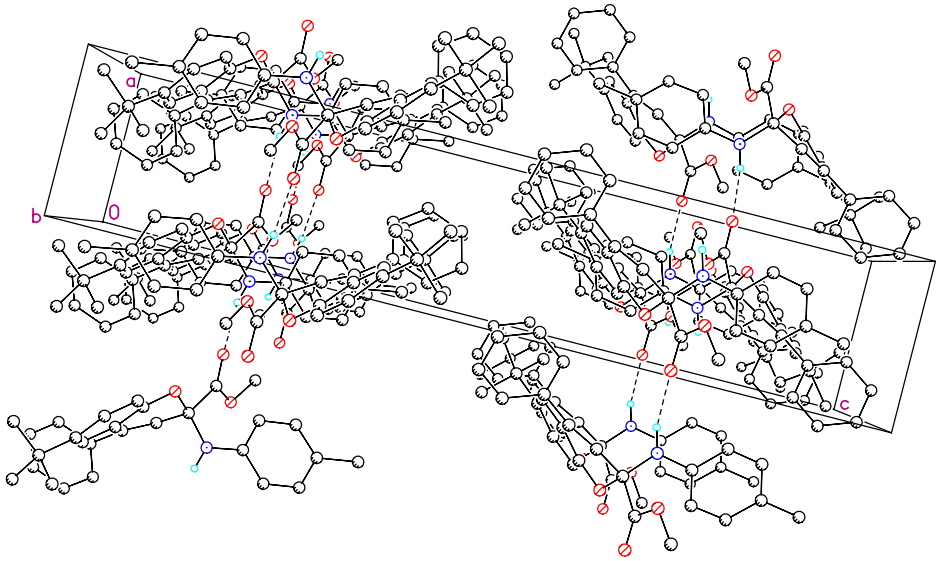


Table 1 Crystal data and structure refinement for **6a**

Identification code	**6a**
Empirical formula	C28 H29 N O3
Formula weight	427.52
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 6.0368(12) A alpha = 90 deg.
	b = 13.398(3) A beta = 90 deg.
	c = 29.789(6) A gamma = 90 deg.
Volume	2409.3(8) A^3
Z, Calculated density	4, 1.179 Mg/m^3
Absorption coefficient	0.076 mm^-1
F(000)	912
Crystal size	0.75 x 0.28 x 0.08 mm
Theta range for data collection	1.37 to 27.47 deg.
Limiting indices	-6<=h<=7, -16<=k<=17, -36<=l<=38
Reflections collected / unique	18931 / 3133 [R(int) = 0.0473]
Completeness to theta = 27.47	98.7 %
Absorption correction	Empirical
Max. and min. transmission	0.9943 and 0.9455
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3133 / 0 / 289
Goodness-of-fit on F^2	1.010
Final R indices [I>2sigma(I)]	R1 = 0.0436, wR2 = 0.1095
R indices (all data)	R1 = 0.0698, wR2 = 0.1307
Absolute structure parameter	-1(2)
Largest diff. peak and hole	0.314 and -0.323 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **6a**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	1746(4)	6238(2)	2461(1)	67(1)
O(2)	4541(3)	7217(2)	2267(1)	75(1)
O(3)	1963(3)	8528(2)	1882(1)	55(1)
N(1)	-855(4)	7980(2)	2380(1)	50(1)
C(1)	3279(6)	5543(3)	2660(1)	82(1)
C(2)	2611(5)	7043(3)	2274(1)	50(1)
C(3)	783(4)	7680(2)	2062(1)	46(1)
C(4)	-370(5)	7120(2)	1692(1)	47(1)
C(5)	-1201(5)	7610(2)	1345(1)	44(1)
C(6)	-2527(5)	7106(2)	989(1)	47(1)
C(7)	-4513(6)	6663(3)	1092(1)	73(1)
C(8)	-5736(7)	6193(3)	759(2)	98(1)
C(9)	-4962(10)	6170(3)	332(2)	98(2)
C(10)	-2996(9)	6592(3)	226(1)	83(1)
C(11)	-1763(6)	7072(2)	554(1)	60(1)
C(12)	-850(5)	8698(2)	1314(1)	47(1)
C(13)	-2010(5)	9316(2)	1025(1)	49(1)
C(14)	-1614(5)	10339(2)	1001(1)	52(1)
C(15)	42(6)	10714(3)	1278(1)	65(1)
C(16)	1204(6)	10117(2)	1568(1)	65(1)
C(17)	759(5)	9112(2)	1592(1)	50(1)
C(18)	-2899(6)	11035(2)	689(1)	57(1)
C(19)	-4033(7)	11854(3)	967(1)	81(1)
C(20)	-1316(7)	11523(3)	356(1)	82(1)
C(21)	-4716(7)	10494(2)	429(1)	71(1)
C(22)	-391(5)	8334(2)	2813(1)	44(1)
C(23)	1589(5)	8786(2)	2925(1)	54(1)
C(24)	1931(6)	9119(2)	3359(1)	56(1)
C(25)	378(6)	9027(2)	3688(1)	53(1)
C(26)	-1626(6)	8598(2)	3569(1)	59(1)
C(27)	-2008(5)	8243(2)	3140(1)	53(1)
C(28)	802(8)	9345(2)	4168(1)	74(1)

Table 3. Bond lengths [A] and angles [deg] for **6a**.

O(1)-C(2)	1.322(4)
O(1)-C(1)	1.440(4)
O(2)-C(2)	1.189(3)
O(3)-C(17)	1.373(3)
O(3)-C(3)	1.444(3)
N(1)-C(22)	1.403(3)
N(1)-C(3)	1.429(3)
C(2)-C(3)	1.531(4)
C(3)-C(4)	1.503(4)
C(4)-C(5)	1.321(4)
C(5)-C(12)	1.476(4)
C(5)-C(6)	1.492(4)
C(6)-C(7)	1.372(5)
C(6)-C(11)	1.375(4)
C(7)-C(8)	1.386(5)
C(8)-C(9)	1.358(7)
C(9)-C(10)	1.352(7)
C(10)-C(11)	1.387(5)
C(12)-C(13)	1.384(4)
C(12)-C(17)	1.393(4)
C(13)-C(14)	1.394(4)
C(14)-C(15)	1.390(4)
C(14)-C(18)	1.527(4)
C(15)-C(16)	1.371(5)
C(16)-C(17)	1.375(4)
C(18)-C(20)	1.525(5)
C(18)-C(21)	1.527(5)
C(18)-C(19)	1.536(4)
C(22)-C(23)	1.380(4)
C(22)-C(27)	1.384(4)
C(23)-C(24)	1.383(4)
C(24)-C(25)	1.363(5)
C(25)-C(26)	1.386(5)
C(25)-C(28)	1.514(4)
C(26)-C(27)	1.381(4)
C(2)-O(1)-C(1)	116.6(2)

C(17)-O(3)-C(3)	114.9(2)
C(22)-N(1)-C(3)	124.6(2)
O(2)-C(2)-O(1)	123.7(3)
O(2)-C(2)-C(3)	126.1(3)
O(1)-C(2)-C(3)	110.2(2)
N(1)-C(3)-O(3)	111.5(2)
N(1)-C(3)-C(4)	107.9(2)
O(3)-C(3)-C(4)	110.5(2)
N(1)-C(3)-C(2)	112.4(2)
O(3)-C(3)-C(2)	103.7(2)
C(4)-C(3)-C(2)	111.0(2)
C(5)-C(4)-C(3)	120.0(3)
C(4)-C(5)-C(12)	119.1(3)
C(4)-C(5)-C(6)	122.3(3)
C(12)-C(5)-C(6)	118.6(2)
C(7)-C(6)-C(11)	119.3(3)
C(7)-C(6)-C(5)	120.4(3)
C(11)-C(6)-C(5)	120.3(3)
C(6)-C(7)-C(8)	120.2(4)
C(9)-C(8)-C(7)	119.8(4)
C(10)-C(9)-C(8)	120.8(4)
C(9)-C(10)-C(11)	120.0(4)
C(6)-C(11)-C(10)	120.0(4)
C(13)-C(12)-C(17)	119.0(3)
C(13)-C(12)-C(5)	123.9(3)
C(17)-C(12)-C(5)	117.1(3)
C(12)-C(13)-C(14)	122.2(3)
C(15)-C(14)-C(13)	116.6(3)
C(15)-C(14)-C(18)	120.4(3)
C(13)-C(14)-C(18)	123.0(3)
C(16)-C(15)-C(14)	122.1(3)
C(15)-C(16)-C(17)	120.3(3)
O(3)-C(17)-C(16)	119.2(3)
O(3)-C(17)-C(12)	121.1(3)
C(16)-C(17)-C(12)	119.7(3)
C(20)-C(18)-C(21)	108.8(3)
C(20)-C(18)-C(14)	109.8(3)
C(21)-C(18)-C(14)	112.6(2)
C(20)-C(18)-C(19)	108.9(3)
C(21)-C(18)-C(19)	107.0(3)
C(14)-C(18)-C(19)	109.6(3)

C(23)-C(22)-C(27)	118.7(3)
C(23)-C(22)-N(1)	122.9(3)
C(27)-C(22)-N(1)	118.5(3)
C(22)-C(23)-C(24)	119.8(3)
C(25)-C(24)-C(23)	122.7(3)
C(24)-C(25)-C(26)	116.9(3)
C(24)-C(25)-C(28)	122.6(3)
C(26)-C(25)-C(28)	120.5(3)
C(27)-C(26)-C(25)	121.7(3)
C(26)-C(27)-C(22)	120.1(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **6a**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
O(1)	48(1)	76(2)	76(1)	21(1)	-9(1)	-7(1)
O(2)	33(1)	101(2)	90(2)	8(2)	-5(1)	-10(1)
O(3)	43(1)	73(1)	50(1)	8(1)	-8(1)	-23(1)
N(1)	30(1)	73(2)	46(1)	-6(1)	-4(1)	-9(1)
C(1)	71(2)	86(2)	90(3)	19(2)	-13(2)	7(2)
C(2)	36(2)	74(2)	41(2)	-7(2)	-1(1)	-8(2)
C(3)	34(1)	62(2)	41(2)	1(1)	-3(1)	-14(1)
C(4)	40(1)	56(2)	46(2)	-4(1)	-4(1)	-13(2)
C(5)	40(1)	51(2)	40(2)	-6(1)	-2(1)	-8(1)
C(6)	50(2)	44(2)	45(2)	-4(1)	-12(1)	-1(1)
C(7)	54(2)	91(3)	74(2)	-17(2)	-8(2)	-17(2)
C(8)	67(3)	107(3)	120(4)	-21(3)	-31(3)	-28(3)
C(9)	123(4)	75(3)	95(3)	-20(2)	-66(3)	-4(3)
C(10)	130(4)	67(2)	51(2)	-12(2)	-31(3)	22(3)
C(11)	75(2)	59(2)	47(2)	1(2)	-12(2)	3(2)
C(12)	44(2)	56(2)	41(2)	-3(1)	1(1)	-10(2)
C(13)	45(2)	54(2)	47(2)	-9(1)	-4(2)	-8(2)

C(14)	53(2)	53(2)	49(2)	-7(1)	6(2)	-7(2)
C(15)	71(2)	56(2)	68(2)	1(2)	-1(2)	-22(2)
C(16)	60(2)	68(2)	66(2)	-1(2)	-9(2)	-32(2)
C(17)	43(2)	65(2)	43(2)	3(1)	-1(1)	-19(2)
C(18)	59(2)	51(2)	63(2)	-5(2)	6(2)	3(2)
C(19)	78(3)	64(2)	100(3)	-18(2)	12(2)	4(2)
C(20)	87(3)	75(2)	84(2)	21(2)	16(2)	6(2)
C(21)	76(2)	69(2)	68(2)	-4(2)	-12(2)	15(2)
C(22)	39(1)	48(2)	46(2)	2(1)	-4(1)	0(1)
C(23)	43(2)	69(2)	51(2)	-6(2)	-2(2)	-12(2)
C(24)	53(2)	56(2)	59(2)	-10(2)	-10(2)	-7(2)
C(25)	67(2)	42(2)	49(2)	-4(1)	-7(2)	7(2)
C(26)	64(2)	62(2)	50(2)	0(2)	11(2)	-4(2)
C(27)	44(2)	59(2)	56(2)	1(2)	0(2)	-8(2)
C(28)	103(3)	64(2)	56(2)	-16(2)	-11(2)	5(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **6a**.

	x	y	z	U(eq)
H(1A)	-2222	7940	2301	60
H(1B)	2476	4992	2786	123
H(1C)	4107	5872	2892	123
H(1D)	4277	5301	2434	123
H(4A)	-498	6429	1707	57
H(7A)	-5038	6677	1385	88
H(8A)	-7084	5895	829	118
H(9A)	-5793	5859	109	117
H(10A)	-2470	6561	-67	99
H(11A)	-421	7371	480	72
H(13A)	-3090	9038	840	59
H(15A)	373	11391	1266	78
H(16A)	2297	10394	1750	77
H(19A)	-2940	12207	1140	121
H(19B)	-5095	11556	1166	121

H(19C)	-4773	12312	770	121
H(20A)	-607	11016	179	122
H(20B)	-214	11896	517	122
H(20C)	-2129	11963	163	122
H(21A)	-4065	9979	248	106
H(21B)	-5477	10961	239	106
H(21C)	-5748	10202	636	106
H(23A)	2688	8865	2709	65
H(24A)	3277	9419	3429	67
H(26A)	-2742	8547	3783	70
H(27A)	-3355	7943	3071	63
H(28A)	2266	9619	4192	112
H(28B)	674	8776	4363	112
H(28C)	-265	9840	4254	112

Table 6. Hydrogen bonds for **6a** [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...O(2)#1	0.86	2.18	2.981(3)	154.0

Symmetry transformations used to generate equivalent atoms:
#1 x-1,y,z